KARL SVOZIL

MATHEMATICAL METH-ODS OF THEORETICAL PHYSICS

EDITION FUNZL

PUBLISHED BY EDITION FUNZL

First printing, August 2012

Contents

List of Figures

List of Tables

This book is dedicated to the memory of
Prof. Dr.math. Ernst Paul Specker – Amez–Droz,
11.2.1920 – 10.12.2011

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.”

Introduction

THIS IS A FIRST ATTEMPT to provide some written material of a course in mathemathical methods of theoretical physics. I have presented this course to an undergraduate audience at the Vienna University of Technology. Only God knows (see Ref. [1] part one, question 14, article 13; and also Ref. [2], 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.

[1] 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

[2] 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

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 aquisitive. 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.

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 [3]. With regards to formal rigour, there appears to be a rather questionable chain of contempt – all too often theoretical physicists suspiciously look down at the experimentalists, mathematical physicists suspiciously look down at the theoreticians, and mathematicians suspiciously look down at the mathematical physicists. I have even experienced the doubts formal logicians expressed about their collegues in mathematics! For an anectodal evidence, take the claim of a very prominant 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’!”

[3] 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

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 desparate 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 a greater unity in physics; as well as for a greater esteem on "both sides of the same effort;" I am also opting for more pragmatism; one that acknowledges the mutual benefits and oneness of theoretical and empirical physical world perceptions. Schrödinger [4] cites Democritus with arguing against a too great separation of the intellect ($\delta\iota\alpha\nu o\iota\alpha$, dianoia) and the senses ($\alpha\iota\sigma\theta\eta\sigma\epsilon\iota\varsigma$, aitheseis). In fragment D 125 from Galen [5], 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."

[4] Erwin Schrödinger. *Nature and the Greeks*. Cambridge University Press, Cambridge, 1954

[5] Hermann Diels. *Die Fragmente der Vorsokratiker, griechisch und deutsch*. Weidmannsche Buchhandlung, Berlin, 1906. URL http://www.archive.org/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!'

PROFESSOR ERNST SPECKER from the ETH Zürich once remarked that, of the many books of David Hilbert, most of them carry his name first, and the name(s) of his co-author(s) appear 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 densly packed pages, which allegedly none of these authors had really written. It appears to be some sort of collective efforts of scholar 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, affaction, 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 [6], 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.

[6] Imre Lakatos. *Philosophical Papers. 1. The Methodology of Scientific Research Programmes*. Cambridge University Press, Cambridge, 1978

HAVING IN MIND this saddening piece of historic evidence, and for as long as we are here on Earth, let us carry on 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 destroyed by me. You are only* *an instrument."*

Part I:
Metamathematics and Metaphysics

1
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 people muse about the unreasonable effectiveness of mathematics in the natural sciences [1].

Zeno of Elea and Parmenides, for instance, wondered how there can be motion, either in universe which is infinitely divisible, or discrete. Because, in the dense case, 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 [2]?

A related question regards the physical limit state of a hypothetical lamp, considered by Thomson [3], with ever decreasing switching cycles. For the sake of perplexion, take Neils Henrik Abel's verdict denouncing that (Letter to Holmboe, January 16, 1826 [4]), *"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.

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

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

which is just a particular instance of a geometric series (see below) with the common ratio "-1." Here, "A" indicates the Abel sum [5] obtained from a "continuation" of the geometric series, or alternatively, by $s = 1 - s$.

As this shows, formal sums of the Leibniz 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 pro-

[1] 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

[2] 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

[3] James F. Thomson. Tasks and supertasks. *Analysis*, 15:1–13, October 1954

[4] Godfrey Harold Hardy. *Divergent Series*. Oxford University Press, 1949

[5] Godfrey Harold Hardy. *Divergent Series*. Oxford University Press, 1949

posal for infinity machines by Blake [6], p. 651, and Weyl [7], pp. 41-42, which could solve many very difficult problems by searching through unbounded recursively enumerable cases. To achive this physically, ultrarelativistic methods suggest to put observers in "fast orbits" or throw them toward black holes [8].

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 is a typical case in which the metaphysical belief in one's own construction of the world overwhelms critical thinking; and what should be wisely taken as an epistemic finding is taken to be ontologic truth.

The connection between physics and formalism has been debated by Bridgman [9], Feynman [10], and Landauer [11], among many others. The question, for instance, is imminent whether we should take the formalism very serious and literal, using it as a guide to new territories, which might even appear absurd, inconsistent and mind-boggling; just like *Alice's Adventures in Wonderland*. Should we expect that all the wild things formally imaginable have a physical realization?

Note that the formalist Hilbert [12], 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 [13], 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 [14] 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 transforming finite subsets of the original volume through isometries, that is, distance preserving mappings such as translations and rotations. This,

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

[7] Hermann Weyl. *Philosophy of Mathematics and Natural Science*. Princeton University Press, Princeton, NJ, 1949

[8] Itamar Pitowsky. The physical Church-Turing thesis and physical computational complexity. *Iyyun*, 39:81–99, 1990

[9] Percy W. Bridgman. A physicist's second reaction to Mengenlehre. *Scripta Mathematica*, 2:101–117, 224–234, 1934

[10] 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

[11] 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

[12] 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 "Elemente" von M genannt werden) zu einem Ganzen."

[13] Raymond M. Smullyan. *What is the Name of This Book?* Prentice-Hall, Inc., Englewood Cliffs, NJ, 1992a; and Raymond M. Smullyan. *Gödel's Incompleteness Theorems*. Oxford University Press, New York, New York, 1992b

[14] Robert French. The Banach-Tarski theorem. *The Mathematical Intelligencer*, 10:21–28, 1988. ISSN 0343-6993. DOI: 10.1007/BF03023740. URL http://dx.doi.org/10.1007/BF03023740; and Stan Wagon. *The Banach-Tarski Paradox*. Cambridge University Press, Cambridge, 1986

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 [15] has a countable infinity of hotel rooms. It is always capable to acommodate 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 [16].

[15] 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."

[16] 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. For instance, the 4th edition of *Proofs from THE BOOK* [1] 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.

[1] 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

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

[2] 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

[3] 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

[4] 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. Kreisler, 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

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

FOR THOSE OF US with a rather limited amount of storage and memory, and with a lot of troubles and problems, is is quite consolating 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 $(r^a)' = ar^{a-1}$? Most of us would acknowledge to be aware of, and be able and happy to apply, this rule.

LET US JUST LIST some concrete examples of the perplexing varieties of proof methods used today.

For the sake of listing 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: $\sqrt{2}^{\sqrt{2}} \not\in \mathbb{Q}$, then $\sqrt{2}^{\sqrt{2}^{\sqrt{2}}} = 2 \in \mathbb{Q}$.

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 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 transcendential was only found by Gelfond and Schneider in 1934!

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.

A TYPICAL PROOF BY CONTRADICTION is about the irrationality of $\sqrt{2}$.

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, they have no common positive divisor other than 1 or, equivalently, if their greatest common 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 even number is again odd); 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 $\sqrt{2}$.

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 be some revelation, a rare gift, such as seemingly in Srīnivāsa Aiyangār Rāmānujan's case?

THERE EXIST ANCIENT and yet rather intuitive – but sometimes distracting and errorneous – informal notions of proof. An example [6] is the Babylonian notion to "prove" arithmetical statements by considering "large number" cases of algebraic formulae such as (Chapter V of Ref. [7]),

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

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

[6] M. Baaz. Über den allgemeinen gehalt von beweisen. In *Contributions to General Algebra*, volume 6, pages 21–29, Vienna, 1988. Hölder-Pichler-Tempsky

[7] Otto Neugebauer. *Vorlesungen über die Geschichte der antiken mathematischen Wissenschaften. 1. Band: Vorgriechische Mathematik*. Springer, Berlin, 1934. page 172

"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 complete induction) it is quite all right to go ahead with it.

Another altogether different issue is knowledge acquired by revelation or by some authority. Oracles occur in modern computer science, but only as idealized concepts whose physical realization is highly questionable if not forbidden.

LET US shortly enumerate some proof methods, among others:

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

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 [8], Tarski [9], and Turing [10] put an end to the formalist program. 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

[8] 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

[9] Alfred Tarski. Der Wahrheitsbegriff in den Sprachen der deduktiven Disziplinen. *Akademie der Wissenschaften in Wien. Mathematisch-naturwissenschaftliche Klasse, Akademischer Anzeiger*, 69:9–12, 1932

[10] A. M. Turing. On computable numbers, with an application to the Entscheidungsproblem. *Proceedings of the London Mathematical Society, Series 2*, 42, 43:230–265, 544–546, 1936-7 and 1937. DOI: 10.1112/plms/s2-42.1.230, 10.1112/plms/s2-43.6.544. URL http://dx.doi.org/10.1112/plms/s2-42.1.230,http://dx.doi.org/10.1112/plms/s2-43.6.544

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.

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 them.

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 accidential, accord with the intuition of most experimentalists today. I call it "accidential" 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 to the real numbers [1]. 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.

[1] S. Drobot. *Real Numbers*. Prentice-Hall, Englewood Cliffs, New Jersey, 1964

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 reals is denumerable. (This assumption will yield a contradiction.) That is, the enumeration is a one-to-one function $f : \mathbb{N} \to \mathbb{R}$ (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,

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

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 $r' = 0.d'_1 d'_2 d'_3 \cdots$ 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 [2] 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.

[2] Percy W. Bridgman. A physicist's second reaction to Mengenlehre. *Scripta Mathematica*, 2:101–117, 224–234, 1934

Part II:
Linear vector spaces

4
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.

"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)*

4.1 Basic definitions

In what follows excerpts from Halmos' beautiful treatment "Finite-Dimensional Vector Spaces" will be reviewed [1]. 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 [2] competing for your attention.

The more physically oriented notation in Mermin's book on quantum information theory [3] is adopted. Vectors are typed in bold face. The overline sign stands for complex conjugation; that is, if $a = \Re a + i\Im a$ is a complex number, then $\overline{a} = \Re a - i\Im a$.

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

4.1.1 Fields of real and complex numbers

In physics, scalars are either real or complex numbers and their associated fields. 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*, and denoted by "+" and "·" (often "$a \cdot b$" is identified with the expression "ab" without the center dot) respectively, such that the following axioms hold:

(i) closure of $\mathbb{F}$ under 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 $a(bc) = (ab)c$;

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

[2] 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/linalg.html/book.pdf

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

(iii) commutativity of addition and multiplication: for all a and b in 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 $\frac{1}{b}$, 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

For proofs and additional information see §2 in

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

A *linear vector space* $\langle \mathfrak{V}, +, \cdot, -, 0, 1\rangle$ is a set $\mathfrak{V}$ of elements called *vectors* satisfying certain 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

$$\begin{aligned} (\alpha + \beta)\mathbf{x} &= \alpha\mathbf{x} + \beta\mathbf{x}, \\ \alpha(\mathbf{x} + \mathbf{y}) &= \alpha\mathbf{x} + \alpha\mathbf{y}, \text{ with } \mathbf{x}, \mathbf{y}, \in \mathfrak{V} \text{ and scalars } \alpha, \beta, \end{aligned} \tag{4.1}$$

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;

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

4.2 Linear independence

A set $\mathfrak{S} = \{\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_k\} \subset \mathfrak{V}$ of vectors $\mathbf{x}_i$ in a linear vector space is *linear independent* if no vector can be written as a linear combination of other vectors in this set $\mathfrak{S}$; that is, $\mathbf{x}_i = \sum_{1\le j\le k,\, j\ne i} \alpha_j \mathbf{x}_j$.

Equivalently, linear independence of the vectors in $\mathfrak{B}$ means that no vector in $\mathfrak{S}$ can be written as a linear combinations of others in $\mathfrak{S}$. That is, let $\{\mathbf{x}_1, \ldots, \mathbf{x}_k\}$; if $\sum_{i=1}^{n} \alpha_i \mathbf{x}_i = 0$ implies $\alpha_i = 0$ for each i, then the set $\mathfrak{S} = \{\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_k\}$ is linearly independent.

4.3 Subspace

A nonempty subset $\mathfrak{M}$ of a vector space is a *subspace* or, used synonymuously, 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, the set of all vectors $\mathbf{z} = \mathbf{x} + \mathbf{y}$, with $\mathbf{x} \in \mathfrak{U}$ and $\mathbf{y} \in \mathfrak{V}$.

For proofs and additional information see §10 in
Paul R.. Halmos. *Finite-dimensional Vector Spaces*. Springer, New York, Heidelberg, Berlin, 1974

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

$$\mathfrak{M} = \text{span}(\mathfrak{U}, \mathfrak{V}) = \text{span}(\mathbf{x}, \mathbf{y}) = \{\alpha\mathbf{x} + \beta\mathbf{y} \mid \alpha, \beta \in \mathbb{F}, \mathbf{x} \in \mathfrak{U}, \mathbf{x} \in \mathfrak{V}\}. \tag{4.2}$$

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

For every vector space $\mathfrak{V}$, the set containing the null vector $\{0\}$, and the vector space $\mathfrak{V}$ itself are subspaces of $\mathfrak{V}$.

4.3.1 Scalar or inner product [§61]

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 44) 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 48.

An inner product space is a vector space $\mathfrak{V}$, together with an inner product; that is, with a map $\langle\cdot\mid\cdot\rangle : \mathfrak{V}\times\mathfrak{V}\longrightarrow\mathbb{R}$ or $\mathbb{C}$, in general $\mathbb{F}$, that satisfies the following three axioms for all vectors and all scalars:

(i) Conjugate symmetry: $\langle \mathbf{x}\mid\mathbf{y}\rangle = \overline{\langle \mathbf{y}\mid\mathbf{x}\rangle}$.

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

(ii) Linearity in the first (and second) argument:

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

(ii) Positive-definiteness: $\langle \mathbf{x}\mid\mathbf{x}\rangle\geq 0$; with equality only for $\mathbf{x}=0$.

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

$$\|\mathbf{x}\| = \sqrt{\langle \mathbf{x}\mid\mathbf{x}\rangle} \tag{4.3}$$

One example is the *dot product*

$$\langle \mathbf{x}|\mathbf{y}\rangle = \sum_{i=1}^{n}\overline{x_i}\,y_i \tag{4.4}$$

of two vectors $\mathbf{x}=(x_1,\ldots,x_n)$ and $\mathbf{y}=(y_1,\ldots,y_n)$ in $\mathbb{C}^n$, which, for real Euclidean space, reduces to the well-known dot product $\langle \mathbf{x}|\mathbf{y}\rangle = x_1y_1+\cdots+x_ny_n = \|\mathbf{x}\|\,\|\mathbf{y}\|\cos\angle(\mathbf{x},\mathbf{y})$.

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

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

$$\langle \mathbf{x}|\mathbf{y}\rangle = 0. \tag{4.5}$$

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

$$\mathfrak{E}^\perp = \{\mathbf{x}\mid\langle \mathbf{x}|\mathbf{y}\rangle = 0, \mathbf{x}\in\mathfrak{V}, \forall\mathbf{y}\in\mathfrak{E} \tag{4.6}$$

denote 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 ($\mathfrak{E}$ may be just vectors of an incomplete basis), $\mathfrak{E}^\perp$ 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 $\mathfrak{E}$.

See page 37 for a definition of subspace.

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 $(0,1)$.

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 equipped with vector addition, scalar multiplication, and some scalar product. Furthermore, *closure* is an additional requirement, but nobody has made operational sense of that so far: If $\mathbf{x}_n \in \mathfrak{V}$, $n = 1,2,\ldots$, and if $\lim_{n,m\to\infty}(\mathbf{x}_n - \mathbf{x}_m, \mathbf{x}_n - \mathbf{x}_m) = 0$, then there exists an $\mathbf{x} \in \mathfrak{V}$ with $\lim_{n\to\infty}(\mathbf{x}_n - \mathbf{x}, \mathbf{x}_n - \mathbf{x}) = 0$.

Infinite dimensional vector spaces and continuous spectra are nontrivial 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 δ_{ij} defined by

$$\delta_{ij} = \begin{cases} 0, & \text{for } i \neq j; \\ 1, & \text{for } i = j \end{cases}. \tag{4.7}$$

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 [4].

[4] 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

4.4 Basis

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

A vector space is finite dimensional if its basis is finite; that is, its basis contains a finite number of elements.

For proofs and additional information see §7 in

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

4.5 Dimension [§8]

The *dimension* of $\mathfrak{V}$ is the number of elements in $\mathfrak{B}$; all bases $\mathfrak{B}$ contain the same number of elements.

What basis should one choose? 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 it is: some directed quantity. *A priori*, this space, in its most primitive form, is not equipped with a basis, or synonymuously, 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. As for numbers (e.g., by different bases, or by prime decomposition), there exist many "competing" ways to code a vector.

Some of these ways are rather straightforward, such as, in particular, the *Cartesian basis*, or, used synonymuosly, the *standard basis*. Other bases are 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 coordinares in two dimensions, or spherical coordinates in three dimensions – to represent a vector, or, more generally, to code any given physical entity (e.g., tensors, operators) by such bases.

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 distingt outcomes $|\uparrow\rangle = |+\rangle$ *versus* $|\downarrow\rangle = |-\rangle$, and $|H\rangle$ *versus* $|V\rangle$, respectively.

4.6 *Coordinates [§46]*

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.

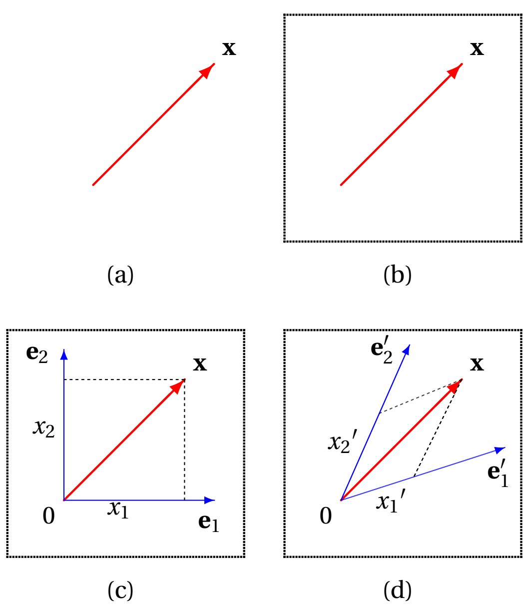


Figure 4.1: Coordinazation of vectors: (a) some primitive vector; (b) some primitive vectors, laid out in some space, denoted by dotted lines (c) vector coordinates x_2 and x_2 of the vector $\mathbf{x} = (x_1, x_2) = x_1\mathbf{e}_1 + x_2\mathbf{e}_2$ in a standard basis; (d) vector coordinates x'_2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

The standard (Cartesian) basis in n-dimensional complex space $\mathbb{C}^n$ is the set of vectors $x_i, i = 1,\ldots,n$, 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 δ_{ij},

Elementary high school tutorials often condition students into believing that the components of the vector “is” the vector, rather then emphasizing that these components *represent* the vector with respect to some (mostly implicitly assumed) basis. A similar problem 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 prjections, the *projector* (i.e., the projection operator; see also page 51) $\mathbf{E_x} = \mathbf{x}^T \otimes \mathbf{x}$ corresponding to a unit (of length 1) vector $\mathbf{x}$ often is identified with where δ_{ij} is the Kronecker delta function

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

Thus,

$$\begin{aligned} \mathbf{e}_1 &= (1,0,\ldots,0), \\ \mathbf{e}_2 &= (0,1,\ldots,0), \\ &\vdots \\ \mathbf{e}_n &= (0,0,\ldots,1). \end{aligned} \tag{4.9}$$

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

$$\mathbf{x} = \sum_{i=1}^{n} x_i \mathbf{e}_i = (x_1, x_2, \ldots, x_n), \tag{4.10}$$

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),

$$\mathbf{x} = (x_1, x_2, \ldots, x_n)^T \cdot (\mathbf{e}_1, \mathbf{e}_2, \ldots, \mathbf{e}_n) = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} (\mathbf{e}_1, \mathbf{e}_2, \ldots, \mathbf{e}_n), \tag{4.11}$$

(the superscript "T" stands for transposition) 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 $\{\mathbf{e}_1, \mathbf{e}_2, \ldots, \mathbf{e}_n\}$; otherwise these numbers lack any meaning whatsoever.

Indeed, with respect to some arbitrary basis $\mathfrak{B} = \{\mathbf{f}_1, \ldots, \mathbf{f}_n\}$ 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

$$\mathbf{x} = \sum_{i=1}^{n} x_i \mathbf{f}_i = (x_1, x_2, \ldots, x_n) \tag{4.12}$$

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 $\mathbf{x} = \sum_{i=1}^{n} y_i \mathbf{f}_i =$

$(y_1, y_2, \ldots, y_n)$; then by subtraction, $0 = \sum_{i=1}^{n}(x_i - y_i)\mathbf{f}_i = (0, 0, \ldots, 0)$. 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 $1 \le i \le n$; hence finally $x_i = y_i$ for all $1 \le i \le n$. 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 $\mathfrak{B} = \{\mathbf{a}_1, \ldots, \mathbf{a}_n\}$ of vectors is *orthonormal* if, whenever for both $\mathbf{a}_i$ and $\mathbf{a}_j$ which are in $\mathfrak{B}$ it follows that

$$\langle \mathbf{a}_i \mid \mathbf{a}_j \rangle = \delta_{ij}. \tag{4.13}$$

Any such set is called *complete* if it is not contained in any larger orthonormal set. Any complete set is a basis.

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 matematics, *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 scalar or inner product $\langle \mathbf{x}|\mathbf{y}\rangle$ of two vectors $\mathbf{x}$ and $\mathbf{y}$ is defined on page 37. In Euclidean space such as $\mathbb{R}^n$, one often identifies the "dot product" $\mathbf{x}\cdot\mathbf{y} = x_1y_1 + \cdots + x_ny_n$ of two vectors $\mathbf{x}$ and $\mathbf{y}$ with their scalar or inner product.

The general method is to start out with the original basis, say, $\{\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \ldots, \mathbf{x}_n\}$, and generate a new orthogonal basis $\{\mathbf{y}_1, \mathbf{y}_2, \mathbf{y}_3, \ldots, \mathbf{y}_n\}$ by

$$\begin{aligned}
\mathbf{y}_1 &= \mathbf{x}_1, \\
\mathbf{y}_2 &= \mathbf{x}_2 - p_{\mathbf{y}_1}(\mathbf{x}_2), \\
\mathbf{y}_3 &= \mathbf{x}_3 - p_{\mathbf{y}_1}(\mathbf{x}_3) - p_{\mathbf{y}_2}(\mathbf{x}_3), \\
&\vdots \\
\mathbf{y}_n &= \mathbf{x}_n - \textstyle\sum_{i=1}^{n-1} p_{\mathbf{y}_i}(\mathbf{x}_n),
\end{aligned} \tag{4.14}$$

where

$$p_{\mathbf{y}}(\mathbf{x}) = \frac{\langle \mathbf{x}|\mathbf{y}\rangle}{\langle \mathbf{y}|\mathbf{y}\rangle}\mathbf{y}, \text{ and } p_{\mathbf{y}}^{\perp}(\mathbf{x}) = \mathbf{x} - \frac{\langle \mathbf{x}|\mathbf{y}\rangle}{\langle \mathbf{y}|\mathbf{y}\rangle}\mathbf{y} \tag{4.15}$$

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,

$$\begin{aligned}
&p_{\mathbf{y}}^2(\mathbf{x}) = p_{\mathbf{y}}(p_{\mathbf{y}}(\mathbf{x})) = \tfrac{\langle \mathbf{x}|\mathbf{y}\rangle}{\langle \mathbf{y}|\mathbf{y}\rangle}\tfrac{\langle \mathbf{y}|\mathbf{y}\rangle}{\langle \mathbf{y}|\mathbf{y}\rangle}\mathbf{y} = p_{\mathbf{y}}(\mathbf{x}), \\
&(p_{\mathbf{y}}^{\perp})^2(\mathbf{x}) = p_{\mathbf{y}}^{\perp}(p_{\mathbf{y}}^{\perp}(\mathbf{x})) = \mathbf{x} - \tfrac{\langle \mathbf{x}|\mathbf{y}\rangle}{\langle \mathbf{y}|\mathbf{y}\rangle}\mathbf{y} - \left(\tfrac{\langle \mathbf{x}|\mathbf{y}\rangle}{\langle \mathbf{y}|\mathbf{y}\rangle} - \tfrac{\langle \mathbf{x}|\mathbf{y}\rangle\langle \mathbf{y}|\mathbf{y}\rangle}{\langle \mathbf{y}|\mathbf{y}\rangle^2}\right)\mathbf{y}, = p_{\mathbf{y}}^{\perp}(\mathbf{x}), \\
&p_{\mathbf{y}}(p_{\mathbf{y}}^{\perp}(\mathbf{x})) = p_{\mathbf{y}}^{\perp}(p_{\mathbf{y}}(\mathbf{x})) = \tfrac{\langle \mathbf{x}|\mathbf{y}\rangle}{\langle \mathbf{y}|\mathbf{y}\rangle}\mathbf{y} - \tfrac{\langle \mathbf{x}|\mathbf{y}\rangle\langle \mathbf{y}|\mathbf{y}\rangle}{\langle \mathbf{y}|\mathbf{y}\rangle^2}\mathbf{y} = 0;
\end{aligned} \tag{4.16}$$

see also page 51.

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 [5], 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, 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

$$\mathbf{y}_2 = \mathbf{x}_2 + \lambda \mathbf{y}_1, \tag{4.17}$$

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

$$\langle \mathbf{x}_2 | \mathbf{y}_1 \rangle + \lambda \langle \mathbf{y}_1 | \mathbf{y}_1 \rangle = 0, \tag{4.18}$$

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

$$\lambda = -\frac{\langle \mathbf{x}_2 | \mathbf{y}_1 \rangle}{\langle \mathbf{y}_1 | \mathbf{y}_1 \rangle}. \tag{4.19}$$

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

$$\mathbf{y}_3 = \mathbf{x}_3 + \mu \mathbf{y}_1 + \nu \mathbf{y}_2, \tag{4.20}$$

and require that it is orthogonal to the two previous orthogonal basis vectors $\mathbf{y}_1$ and $\mathbf{y}_2$; that is $\langle \mathbf{y}_1 | \mathbf{y}_3 \rangle = \langle \mathbf{y}_2 | \mathbf{y}_3 \rangle = 0$. As a result,

$$\mu = -\frac{\langle \mathbf{x}_3 | \mathbf{y}_1 \rangle}{\langle \mathbf{y}_1 | \mathbf{y}_1 \rangle}, \quad \nu = -\frac{\langle \mathbf{x}_3 | \mathbf{y}_2 \rangle}{\langle \mathbf{y}_2 | \mathbf{y}_2 \rangle}. \tag{4.21}$$

A generalization of this construction for all the other new base vectors $\mathbf{y}_3, \ldots, \mathbf{y}_n$ is straightforward.

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 *Mutually unbiased bases*

Two orthonormal bases $\{\mathbf{x}_1, \ldots, \mathbf{x}_n\}$ and $\{\mathbf{y}_1, \ldots, \mathbf{y}_n\}$ are said to be *mutually unbiased* if their scalar or inner products are

$$|\langle \mathbf{x}_i | \mathbf{y}_j \rangle|^2 = \frac{1}{n} \tag{4.22}$$

[5] Werner Greub. *Linear Algebra*, volume 23 of *Graduate Texts in Mathematics*. Springer, New York, Heidelberg, fourth edition, 1975

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 whose elements in different bases are maximally apart [6] . Such maximal sets are used in quantum information 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.

[6] 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`; 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/S0219749910006502. URL `http://dx.doi.org/10.1142/S0219749910006502`

Consider, for example, the real plane $\mathbb{R}^2$. There the two bases

$$\begin{aligned} &\{(0,1),(1,0)\} \text{ and} \\ &\{\tfrac{1}{\sqrt{2}}(1,1), \tfrac{1}{\sqrt{2}}(-1,1)\} \end{aligned} \tag{4.23}$$

are mutually unbiased.

For a proof, just form the four inner products.

4.9 Direct sum

For proofs and additional information see §18 in

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

Let $\mathfrak{U}$ and $\mathfrak{V}$ be vector spaces (over the same field, say $\mathbb{C}$). Their *direct sum* $\mathfrak{W} = \mathfrak{U} \oplus \mathfrak{V}$ consist 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

$$(\alpha \mathbf{x}_1 + \beta \mathbf{x}_2, \alpha \mathbf{y}_1 + \beta \mathbf{y}_2) = \alpha(\mathbf{x}_1, \mathbf{y}_1) + \beta(\mathbf{x}_2, \mathbf{y}_2). \tag{4.24}$$

We 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) $\mathfrak{U} \bigcap \mathfrak{V} = \mathfrak{o}$ and $\mathfrak{U} + \mathfrak{V} = \mathfrak{W}$ (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.

4.10 Dual space

For proofs and additional information see §13–15 in

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

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 $\mathbf{x} = (x_1, \ldots, x_n)$, and take $\mathbf{y}(\mathbf{x}) = x_1$.

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

If we adopt a bracket notation "$[\cdot,\cdot]$" for the functional

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

then this "bracket" functional is *bilinear* in its two arguments; that is,

$$[\alpha_1 \mathbf{x}_1 + \alpha_2 \mathbf{x}_2, \mathbf{y}] = \alpha_1 [\mathbf{x}_1, \mathbf{y}] + \alpha_2 [\mathbf{x}_2, \mathbf{y}], \tag{4.27}$$

and

$$[\mathbf{x}, \alpha_1 \mathbf{y}_1 + \alpha_2 \mathbf{y}_2] = \alpha_1 [\mathbf{x}, \mathbf{y}_1] + \alpha_2 [\mathbf{x}, \mathbf{y}_2]. \tag{4.28}$$

The square bracket can be identified with the scalar (dot) product $[\mathbf{x}, \mathbf{y}] = \langle \mathbf{x} \mid \mathbf{y} \rangle$ 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.

If $\mathfrak{V}$ is an n-dimensional vector space, and if $\mathfrak{B} = \{\mathbf{f}_1, \ldots, \mathbf{f}_n\}$ is a basis of $\mathfrak{V}$, and if $\{\alpha_1, \ldots, \alpha_n\}$ 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 $0 \le 1 \le n$.

A constructive proof of this theorem can be given as follows: Since every $\mathbf{x} \in \mathfrak{V}$ can be written as a linear combination $\mathbf{x} = x_1 \mathbf{f}_1 + \cdots + x_n \mathbf{f}_n$ of the base vectors in $\mathfrak{B}$ in a unique way; and since $\mathbf{y}$ is a (bi)linear functional, we obtain

$$[\mathbf{x}, \mathbf{y}] = x_1 [\mathbf{f}_1, \mathbf{y}] + \cdots + x_n [\mathbf{f}_n, \mathbf{y}], \tag{4.29}$$

and uniqueness follows. With $[\mathbf{f}_i, \mathbf{y}] = \alpha_i$ for all $0 \le 1 \le n$, the value of $[\mathbf{x}, \mathbf{y}]$ is determined by $[\mathbf{x}, \mathbf{y}] = x_i \alpha_i + \cdots + x_n \alpha_n$.

4.10.1 Dual basis

We now can define a *dual basis*, or, used synonymuously a *reciprocal basis*. If $\mathfrak{V}$ is an n-dimensional vector space, and if $\mathfrak{B} = \{\mathbf{f}_1, \ldots, \mathbf{f}_n\}$ is a basis of $\mathfrak{V}$, then there is a unique *dual basis* $\mathfrak{B}^* = \{\mathbf{f}_1^*, \ldots, \mathbf{f}_n^*\}$ in the dual vector space $\mathfrak{V}^*$ with the property that

$$[f_i^*, f_j] = \delta_{ij}, \tag{4.30}$$

where δ_{ij} is the Kronecker delta function. More generally, if g is the *metric tensor*, the dual basis is defined by

$$g(\mathbf{f}_i^*, \mathbf{f}_j) = \delta_{ij}. \tag{4.31}$$

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

$$g(\mathbf{f}^j, \mathbf{f}_i) = \delta_i^j. \tag{4.32}$$

In terms of the inner product, the representation of the metric g as outlined and characterized on page 92 with respect to a particular basis $\mathfrak{B} = \{\mathbf{f}_1, \ldots, \mathbf{f}_n\}$ is $g_{ij} = g(\mathbf{f}_i, \mathbf{f}_j) = \langle \mathbf{f}_i \mid \mathbf{f}_j \rangle$. Note that the coordinates g_{ij} of the metric g need not necessarily be positive definite. For example, special relativity uses the "pseudo-Euclidean" metric $g = \mathrm{diag}(+1, +1, +1, -1)$

(or just $g = \text{diag}(+,+,+,-)$), where "diag" stands for the *diagonal matrix* with the arguments in the diagonal.

The dual space $\mathfrak{V}^*$ is n-dimensional.

In a real Euclidean vector space $\mathbb{R}^n$ with the dot product as scalar product, the dual basis of an orthogonal basis is also orthogonal. Moreover, for an orthonormal basis, the bases vectors are uniquely identifiable by $\mathbf{e_i} \longrightarrow \mathbf{e_i}^* = \mathbf{e_i}^T$. This is *not* true for nonorthogonal bases.

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, $g(\mathbf{x},\mathbf{y}) = g(\mathbf{x},\mathbf{y})$ and *nondegenerate*; 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 $||\mathbf{x}-\mathbf{z}|| \leq ||\mathbf{x}-\mathbf{y}|| + ||\mathbf{y}-\mathbf{z}||$.

In a proof by *reductio ad absurdum.* Suppose there exist a vector $\mathbf{e_i}^*$ in the dual basis $\mathfrak{B}^*$ which is not in the "original" ortogonal basis $\mathfrak{B}$; that is, $[\mathbf{e_i}^*, \mathbf{e_j}] = \delta_{ij}$ for all $\mathbf{e_j} \in \mathfrak{B}$. But since $\mathfrak{B}$ is supposed to span the corresponding vector space $\mathfrak{V}$, $\mathbf{e_i}^*$ has to be contained in $\mathfrak{B}$. Moreover, since for a real Euclidean vector space $\mathbb{R}^n$ with the dot product as scalar product, the two products $[\cdot,\cdot] = \langle \cdot \mid \cdot \rangle$ coincide, $\mathbf{e_i}^*$ has to be collinear – for normalized basis vectors even identical – to exactly one element of $\mathfrak{B}$.

For nonorthogonal bases, take the counterexample explicitly mentioned at page 47.

How can one determine the dual basis from a given, not necessarily orthogonal, basis? The tuples of *row vectors* of the basis $\mathfrak{B} = \{\mathbf{f}_1, \ldots, \mathbf{f}_n\}$ can be arranged into a matrix

$$\mathbf{B} = \begin{pmatrix} \mathbf{f}_1 \\ \mathbf{f}_2 \\ \vdots \\ \mathbf{f}_n \end{pmatrix} = \begin{pmatrix} \mathbf{f}_{1,1} & \cdots & \mathbf{f}_{1,n} \\ \mathbf{f}_{2,1} & \cdots & \mathbf{f}_{2,n} \\ \vdots & \vdots & \vdots \\ \mathbf{f}_{n,1} & \cdots & \mathbf{f}_{n,n} \end{pmatrix}. \tag{4.33}$$

Then take the *inverse matrix* $\mathbf{B}^{-1}$, and interprete the *columns vectors* of $\mathbf{B}^{-1}$ as the tuples of the dual basis $\mathfrak{B}^*$.

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

(i) For example, if

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

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

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

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

(ii) If

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

$\alpha_1, \alpha_2, \ldots, \alpha_n \in \mathbb{R}$, is a "dilated" basis in n-dimensional vector space containing unit vectors of norm (or length) α_i, then

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

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

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

4.10.2 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*

$$\mathbf{x} = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix}, \tag{4.34}$$

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

$$\mathbf{x}^* = (x_1^*, x_2^*, \ldots, x_n^*). \tag{4.35}$$

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 [7], Section 11.4),

[7] Hans Havlicek. *Lineare Algebra für Technische Mathematiker*. Heldermann Verlag, Lemgo, second edition, 2008

$$x_i = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} \text{ and } x^i = (x_1^*, x_2^*, \dots, x_n^*). \tag{4.36}$$

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.

The *Einstein summation convention* requires that, when an index variable appears twice in a single term it implies that 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, $x^i = x_i$.

4.10.3 Representation of a functional by inner product

For proofs and additional information see §67 in
Paul R.. Halmos. *Finite-dimensional Vector Spaces*. Springer, New York, Heidelberg, Berlin, 1974

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

$$\mathbf{z}(\mathbf{x}) = [\mathbf{x}, \mathbf{z}] = \langle \mathbf{x} \mid \mathbf{y} \rangle \tag{4.37}$$

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

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

4.11 Tensor product

4.11.1 Definition

For proofs and additional information see §24 in
Paul R.. Halmos. *Finite-dimensional Vector Spaces*. Springer, New York, Heidelberg, Berlin, 1974

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 avery $\mathbf{y} \in \mathfrak{U}$ there corresponds a tensor product $\mathbf{z} = \mathbf{x} \otimes \mathbf{y} \in \mathfrak{V} \otimes \mathfrak{U}$ which is bilinear in both factors.

If $\mathfrak{A} = \{\mathbf{f}_1, \ldots, \mathbf{f}_n\}$ and $\mathfrak{B} = \{\mathbf{g}_1, \ldots, \mathbf{g}_m\}$ are bases of n- and m- dimensional vector spaces $\mathfrak{V}$ and $\mathfrak{U}$, respectively, then the set $\mathfrak{Z}$ of vectors $\mathbf{z}_{ij} = \mathbf{f}_i \otimes \mathbf{g}_j$ with $i = 1, \ldots n$ and $j = 1, \ldots m$ is a basis of the tensor product $\mathfrak{V} \otimes \mathfrak{U}$.

A generalization to more than one factors is straightforward.

4.11.2 Representation

The tensor product $\mathbf{z} = \mathbf{x} \otimes \mathbf{y}$ 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;

(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 $\mathbf{z} = (x_1\mathbf{y}, x_2\mathbf{y}, \ldots, x_n\mathbf{y}) = (x_1 y_1, x_1 y_2, \ldots, x_n y_n)$. 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.

4.12 Linear transformation

4.12.1 Definition

For proofs and additional information see §32-34 in
Paul R.. Halmos. *Finite-dimensional Vector Spaces*. Springer, New York, Heidelberg, Berlin, 1974

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

$$\mathsf{A}(\alpha\mathbf{x} + \beta\mathbf{y}) = \alpha\mathsf{A}\mathbf{x} + \beta\mathsf{A}\mathbf{y}, \tag{4.38}$$

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

4.12.2 Operations

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

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

The notation $\mathsf{A}^n\mathsf{A}^m = \mathsf{A}^{n+m}$ and $(\mathsf{A}^n)^m = \mathsf{A}^{nm}$, with $\mathsf{A}^1 = \mathsf{A}$ and $\mathsf{A}^0 = \mathsf{1}$ 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 $\mathsf{A}\mathsf{0} = \mathsf{0}\mathsf{A} = \mathsf{0}$, $\mathsf{A}\mathsf{1} = \mathsf{1}\mathsf{A} = \mathsf{A}$, $\mathsf{A}(\mathsf{B} + \mathsf{C}) = \mathsf{A}\mathsf{B} + \mathsf{A}\mathsf{C}$, $(\mathsf{A} + \mathsf{B})\mathsf{C} = \mathsf{A}\mathsf{C} + \mathsf{B}\mathsf{C}$, and $\mathbf{A}(\mathbf{BC}) = (\mathbf{AB})\mathbf{C}$. 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 $\mathbf{AA}^{-1} = \mathbf{A}^{-1}\mathbf{A} = \mathbf{I}$.

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

$$[\mathbf{A}, \mathbf{B}] = \mathbf{AB} - \mathbf{BA}. \tag{4.39}$$

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

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

$$p(\mathbf{A}) = \alpha_0 \mathbf{1} + \alpha_1 \mathbf{A}^1 + \alpha_2 \mathbf{A}^2 + \cdots + \alpha_n \mathbf{A}^n = \sum_{i=0}^{n} \alpha_i \mathbf{A}^i. \tag{4.40}$$

The Baker-Hausdorff formula

$$e^{i\mathbf{A}}\mathbf{B}e^{-i\mathbf{A}} = B + i[\mathbf{A}, \mathbf{B}] + \frac{i^2}{2!}[\mathbf{A}, [\mathbf{A}, \mathbf{B}]] + \cdots \tag{4.41}$$

for two arbitrary noncommutative linear operators $\mathbf{A}$ and $\mathbf{B}$ is mentioned without proof (cf. Messiah, *Quantum Mechanics, Vol. 1* [8]).

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

$$e^{\mathbf{A}} e^{\mathbf{B}} = e^{\mathbf{A} + \mathbf{B} + \frac{1}{2}[\mathbf{A}, \mathbf{B}]}. \tag{4.42}$$

[8] A. Messiah. *Quantum Mechanics*, volume I. North-Holland, Amsterdam, 1962

4.12.3 Linear transformations as matrices

Due to linearity, there is a close connection between a matrix defined by an n-by-n square array

$$A = \langle i|A|j\rangle = a_{ij} = \begin{pmatrix} \alpha_{11} & \alpha_{12} & \cdots & \alpha_{1n} \\ \alpha_{21} & \alpha_{22} & \cdots & \alpha_{2n} \\ \vdots & \vdots & \cdots & \vdots \\ \alpha_{n1} & \alpha_{n2} & \cdots & \alpha_{nn} \end{pmatrix} \tag{4.43}$$

containing n^2 entries, also called matrix coefficients or matrix coordinates, α_{ij} and a linear transformation $\mathbf{A}$, encoded with respect to a particular basis $\mathfrak{B}$. This can be well understood in terms of transformations of the basis elements, as every vector is a unique linear combination of these basis elements; more explicitly, see the *Ansatz* $\mathbf{y}_i = \mathbf{A}\mathbf{x}_i$ in Eq. (4.50) below.

Let $\mathfrak{V}$ be an n-dimensional vector space; let $\mathfrak{B} = \{\mathbf{f}_1, \mathbf{f}_2, \ldots, \mathbf{f}_n\}$ be any basis of $\mathfrak{V}$, and let $\mathbf{A}$ be a linear transformation on $\mathfrak{V}$. Because every vector is a linear combination of the basis vectors $\mathbf{f}_i$, it is possible to define some matrix coefficients or coordinates α_{ij} such that

$$\mathbf{A}\mathbf{f}_j = \sum_i \alpha_{ij} \mathbf{f}_i \tag{4.44}$$

for all $j = 1, \ldots, n$. Again, note that this definition of a *transformation matrix* is tied up with a basis.

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 [9]:

$$\begin{aligned}\sigma_1 = \sigma_x &= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},\\ \sigma_2 = \sigma_y &= \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix},\\ \sigma_1 = \sigma_z &= \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.\end{aligned} \tag{4.45}$$

[9] Leonard I. Schiff. *Quantum Mechanics.* McGraw-Hill, New York, 1955

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

$$\begin{aligned}[\sigma_1, \sigma_3] &= \sigma_1\sigma_3 - \sigma_3\sigma_1\\ &= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} - \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\\ &= 2\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \neq \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}.\end{aligned} \tag{4.46}$$

4.13 *Projector or Projection*

4.13.1 *Definition*

For proofs and additional information see §41 in

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

If $\mathfrak{V}$ is the direct sum of some subspaces $\mathfrak{M}$ and $\mathfrak{N}$ so that verey $\mathbf{z} \in \mathfrak{V}$ 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 *projector*, or, uses synonymuosly, *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 projector on $\mathfrak{N}$ along $\mathfrak{M}$.

A linear transformation $\mathbf{E}$ is a projector if and only if it is idempotent; that is, $\mathbf{E}\mathbf{E} = \mathbf{E}$.

For a proof note that, if $\mathbf{E}$ is the projector 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 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 projector – is more difficult to prove. For this proof we refer to the literature; e.g., Halmos [10].

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

We also mention without proof that a linear transformation $\mathbf{E}$ is a projector if and only if $\mathbf{1} - \mathbf{E}$ is a projector. 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 projector on $\mathfrak{M}$ along $\mathfrak{N}$, then $\mathbf{1} - \mathbf{E}$ is the projector on $\mathfrak{N}$ along $\mathfrak{M}$.

4.13.2 *Construction of projectors from unit vectors*

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

Let $\mathbf{x}$ be the coordinates of a unit vector; that is $\|\mathbf{x}\| = 1$. Then the dyadic or tensor product (also in Dirac's bra and ket notation)

$$\begin{aligned}
\mathsf{E}_{\mathbf{x}} &= \mathbf{x} \otimes \mathbf{x}^T = |\mathbf{x}\rangle\langle\mathbf{x}| \\
&= \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} (x_1, x_2, \dots, x_n) \\
&= \begin{pmatrix} x_1(x_1, x_2, \dots, x_n) \\ x_2(x_1, x_2, \dots, x_n) \\ \vdots \\ x_n(x_1, x_2, \dots, x_n) \end{pmatrix} \\
&= \begin{pmatrix} x_1x_1 & x_1x_2 & \cdots & x_1x_n \\ x_2x_1 & x_2x_2 & \cdots & x_2x_n \\ \vdots & \vdots & \vdots & \vdots \\ x_nx_1 & x_nx_2 & \cdots & x_nx_n \end{pmatrix}
\end{aligned} \tag{4.47}$$

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

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

$$\mathsf{E}_{\mathbf{x}} = \frac{\mathbf{x} \otimes \mathbf{x}^T}{\langle \mathbf{x} \mid \mathbf{x} \rangle} = \frac{|\mathbf{x}\rangle\langle\mathbf{x}|}{\langle \mathbf{x} \mid \mathbf{x} \rangle} \tag{4.48}$$

This construction is related to $p_{\mathbf{x}}$ on page 42 by $p_{\mathbf{x}}(\mathbf{y}) = \mathsf{E}_{\mathbf{x}}\mathbf{y}$.

For a proof, let $\mathsf{E}_{\mathbf{x}} = \mathbf{x} \otimes \mathbf{x}^T$, then

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

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

$$\mathbf{E_x} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}(1,0) = \begin{pmatrix} 1(1,0) \\ 0(1,0) \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix},$$

and

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

4.14 *Change of basis*

For proofs and additional information see §46 in

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

Let $\mathfrak{V}$ be an n-dimensional vector space land let $\mathfrak{X} = \{\mathbf{x}_1, \ldots, \mathbf{x}_n\}$ and $\mathfrak{Y} = \{\mathbf{y}_1, \ldots, \mathbf{y}_n\}$ be two bases in $\mathfrak{V}$.

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

$$\mathbf{x} = \sum_{i=1}^{n} x^i \mathbf{x}_i = \sum_{i=1}^{n} y^i \mathbf{y}_i, \tag{4.49}$$

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

What is the relation between the coordinates x^i and y^i? Suppose that, as an *Ansatz*, we define a linear transformation between the corresponding vectors of the bases $\mathfrak{X}$ and $\mathfrak{Y}$ by

$$\mathbf{y}_i = \mathbf{A}\mathbf{x}_i, \tag{4.50}$$

for all $i = 1, \ldots, n$. Note that somewhat "hidden" in Eq. (4.50) there is a matrix multiplication which can be made explicit: let a_{ij} be the matrix components corresponding to $\mathbf{A}$ in the basis $\mathfrak{X}$; then

$$\mathbf{y}_j = \mathbf{A}\mathbf{x}_j = \sum_{i=1}^{n} a_{ij}\mathbf{x}_i. \tag{4.51}$$

Here, the subscript "j" refers to the jth coordinate of $\mathbf{y}$, whereas in Eq. (4.50) the subscript "j" refers to the jth vectors $\mathbf{x}_j$ and $\mathbf{y}_i$ in the two bases $\mathfrak{X}$ and $\mathfrak{Y}$, respectively.

Then, since

$$\mathbf{x} = \sum_{j=1}^{n} y^j \mathbf{y}_j = \sum_{j=1}^{n} y^j \mathbf{A}\mathbf{x}_j = \sum_{j=1}^{n} y^j \sum_{i=1}^{n} a_{ij}\mathbf{x}_i = \sum_{i=1}^{n}\left(\sum_{j=1}^{n} a_{ij} y^j\right)\mathbf{x}_i;$$

and hence by comparison of the coefficients in Eq. (4.49),

$$x^i = \sum_{j=1}^{n} a_{ij} y^j. \tag{4.52}$$

4.15 Rank

The (column or row) *rank*, $\rho(\mathbf{A})$ of a linear transformation $\mathbf{A}$ in an n-dimensional vector space $\mathfrak{V}$ is the maximum number of linearly independent (column or, without proof, equivalently, row) vectors of the associated n-by-n square matrix a_{ij}.

4.16 Determinant

4.16.1 Definition

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* recursively.

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 ith row and jth 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

$$A_{ij} = (-1)^{i+j} M_{ij}. \tag{4.53}$$

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

$$\det A = \sum_{j=1}^{n} a_{ij} A_{ij} = \sum_{i=1}^{n} a_{ij} A_{ij} \tag{4.54}$$

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

4.16.2 Properties

The following properties of determinants are mentioned 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) $\det(A^T) = \det A$.

(iv) The determinant $\det A$ of a matrix A is non-zero 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 $\det(A^{-1}) = (\det A)^{-1}$.

(v) Multiplication of any row or column with a factor α results in a determinant which is α times the original determinant.

4.17 Trace

4.17.1 Definition

The German word for trace is *Spur*.

The *trace* of an n-by-n square matrix $A = a_{ij}$, denoted by TrA, 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),

$$\text{Tr}A = a_{11} + a_{22} + \cdots + a_{nn} = \sum_{i=1}^{n} a_{ii} = \sum_{i=1}^{n} \langle i|A|i\rangle. \tag{4.55}$$

4.17.2 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) $\text{Tr}(AB) = \text{Tr}(BA)$;

(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;

(vii) $\det(e^A) = e^{\text{Tr}A}$;

(viii) the trace is the derivative of the determinant at the identity;

(xi) the complex conjugate of the trace of an operator is equal to the trace of its adjoint; that is $\overline{(\text{Tr}A)} = \text{Tr}(A^\dagger)$;

(xi) the trace is invariant under rotations of the basis and under cyclic permutations.

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

4.18 Adjoint

4.18.1 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 $\mathbf{y}'(\mathbf{x}) = [\mathbf{x}, \mathbf{y}'] = [\mathbf{A}\mathbf{x}, \mathbf{y}]$ Let the *adjoint* transformation $\mathbf{A}^\dagger$ be defined by

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

$$[\mathbf{x}, \mathbf{A}^\dagger \mathbf{y}] = [\mathbf{A}\mathbf{x}, \mathbf{y}]. \tag{4.56}$$

4.18.2 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)

$$\mathbf{A}^{\dagger\dagger} = \mathbf{A}. \tag{4.57}$$

4.18.3 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 48) 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

$$\begin{aligned}
&[\mathbf{Ax}, \mathbf{z}] \\
&\quad = \langle \mathbf{Ax} \mid \mathbf{y} \rangle \\
&\quad = \overline{\langle \mathbf{y} \mid \mathbf{Ax} \rangle} \\
&\quad = y_i \overline{A_{ij}} x_j \\
&\quad = y_i \overline{A}^T_{ji} x_j \\
&\qquad = x \overline{A}^T y \\
&= [\mathbf{x}, \mathbf{A}^\dagger \mathbf{z}] \\
&\quad = \langle \mathbf{x} \mid \mathbf{A}^\dagger \mathbf{y} \rangle \\
&\quad = x_i A^\dagger_{ij} y_j \\
&\qquad = x A^\dagger y,
\end{aligned} \tag{4.58}$$

and hence

$$A^\dagger = (\overline{A})^T = \overline{A^T}, \text{ or } A^\dagger_{ij} = \overline{A}_{ji}. \tag{4.59}$$

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

4.19 Self-adjoint transformation

The following definition yields some analogy to real numbers as compared to complex numbers ("a complex number z is real if $\overline{z} = z$"), 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

$$\mathbf{A}^\dagger = \mathbf{A}. \tag{4.60}$$

In terms of matrices, a matrix A corresponding to an operator $\mathbf{A}$ in some fixed basis is self-adjoint if

$$A^\dagger = (\overline{A_{ij}})^T = \overline{A_{ij}} = A_{ij} = A. \tag{4.61}$$

More generally, if the matrix corresponding to $\mathbf{A}$ in some basis $\mathfrak{B}$ is A_{ij}, then the matrix corresponding to $\mathbf{A}^*$ with respect to the dual basis $\mathfrak{B}^*$ is $\overline{(A_{ij})}^T$.

In real inner product spaces, the usual word for a self-adjoint transformation is *symmetric* transformation. In complex inner product spaces, the usual word for self-adjoint is *Hermitian* transformation.

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

$$\sigma_1 = \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_1 = \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{4.62}$$

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

The following operators are not self-adjoint:

$$\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \begin{pmatrix} 1 & 1 \\ 0 & 0 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ i & 0 \end{pmatrix}, \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix}. \tag{4.63}$$

4.20 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 $\langle \mathbf{Ax} \mid \mathbf{x} \rangle \geq 0$ for all $\mathbf{x} \in \mathfrak{V}$. If $\langle \mathbf{Ax} \mid \mathbf{x} \rangle = 0$ implies $\mathbf{x} = 0$, $\mathbf{A}$ is called *strictly positive*.

4.21 Unitary transformations and isometries

4.21.1 Definition

For proofs and additional information see §73 in
Paul R.. Halmos. *Finite-dimensional Vector Spaces*. Springer, New York, Heidelberg, Berlin, 1974

Note that a complex number z has absolute value one if $\overline{z} = 1/z$, or $z\overline{z} = 1$. In analogy to this "modulus one" behavior, consider *unitary transformations*, or, used synonymuously, *isometries* $\mathbf{U}$ for which

$$\mathbf{U}^* = \mathbf{U}^\dagger = \mathbf{U}^{-1}, \text{ or } \mathbf{U}\mathbf{U}^\dagger = \mathbf{U}^\dagger\mathbf{U} = \mathbf{I}. \tag{4.64}$$

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

(i) $\langle \mathbf{Ux} \mid \mathbf{Uy} \rangle = \langle \mathbf{x} \mid \mathbf{y} \rangle$ for all $\mathbf{x}, \mathbf{y} \in \mathfrak{V}$;

(ii) $\|\mathbf{Ux}\| = \|\mathbf{x}\|$ for all $\mathbf{x}, \mathbf{y} \in \mathfrak{V}$;

4.21.2 Characterization of change of orthonormal basis

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

4.21.3 Characterization in terms of orthonormal basis

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

This can be readily verified [11] by writing 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

$$\mathsf{U}_{ef} = \sum_{i=1}^{n} \mathbf{e}_i^\dagger \mathbf{f}_i = \sum_{i=1}^{n} |\mathbf{e}_i\rangle\langle\mathbf{f}_i|. \tag{4.65}$$

[11] J. Schwinger. Unitary operators bases. In *Proceedings of the National Academy of Sciences (PNAS)*, volume 46, pages 570–579, 1960. DOI: 10.1073/pnas.46.4.570. URL http://dx.doi.org/10.1073/pnas.46.4.570

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

$$\begin{aligned} &\mathbf{e}_k \mathsf{U}_{ef} \\ &\quad = \mathbf{e}_k \textstyle\sum_{i=1}^{n} \mathbf{e}_i^\dagger \mathbf{f}_i \\ &\quad = \textstyle\sum_{i=1}^{n} (\mathbf{e}_k \mathbf{e}_i^\dagger) \mathbf{f}_i \\ &\quad = \textstyle\sum_{i=1}^{n} \delta_{ki} \mathbf{f}_i \\ &\quad = \mathbf{f}_k. \end{aligned} \tag{4.66}$$

In a similar wey we find that

$$\begin{aligned} \mathsf{U}_{ef} \mathbf{f}_k^\dagger &= \mathbf{e}_k^\dagger, \\ \mathbf{f}_k \mathsf{U}_{fe} &= \mathbf{f}_k, \\ \mathsf{U}_{fe} \mathbf{e}_k^\dagger &= \mathbf{f}_k^\dagger. \end{aligned} \tag{4.67}$$

Moreover,

$$\begin{aligned} &\mathsf{U}_{ef} \mathsf{U}_{fe} \\ &\quad = \textstyle\sum_{i=1}^{n} \sum_{j=1}^{n} |\mathbf{e}_i\rangle\langle\mathbf{f}_i||\mathbf{f}_j\rangle\langle\mathbf{e}_j| \\ &\quad = \textstyle\sum_{i=1}^{n} \sum_{j=1}^{n} |\mathbf{e}_i\rangle \delta_{ij} \langle\mathbf{e}_j| \\ &\quad = \textstyle\sum_{i=1}^{n} |\mathbf{e}_i\rangle\langle\mathbf{e}_i| \\ &\quad = \mathbb{I}. \end{aligned} \tag{4.68}$$

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

$$\mathsf{U}_{ef}^\dagger = \sum_{i=1}^{n} (\mathbf{e}_i^\dagger)^\dagger \mathbf{f}_i^\dagger = \mathsf{U}_{fe}, \tag{4.69}$$

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

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

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 U can be written 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

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

$$\mathsf{U} = \begin{pmatrix} \mathbf{f}_1 \\ \mathbf{f}_2 \\ \vdots \\ \mathbf{f}_n \end{pmatrix}. \tag{4.70}$$

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

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

$$\mathsf{U} = \left(\mathbf{f}_1^T, \mathbf{f}_2^T, \cdots, \mathbf{f}_n^T\right). \tag{4.71}$$

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

Of course, any permutation of vectors in $\mathfrak{B}$ would also yield unitary matrices.

4.22 Orthogonal projectors

For proofs and additional information see §75 & 76 in
Paul R.. Halmos. *Finite-dimensional Vector Spaces*. Springer, New York, Heidelberg, Berlin, 1974

A linear transformation E is an orthogonal projector if and only if $\mathsf{E} = \mathsf{E}^2 = \mathsf{E}^*$.

If $\mathsf{E}_1, \mathsf{E}_2, \ldots, \mathsf{E}_n$ are orthogonal projectors, then a necessary and sufficient condition that $\mathsf{E} = \mathsf{E}_1 + \mathsf{E}_2 + \cdots + \mathsf{E}_n$ be an orthogonal projector is that $\mathsf{E}_i \mathsf{E}_j = 0$ whenever $i \neq j$; that is, that all E_i are pairwise orthogonal.

4.23 Proper value or eigenvalue

For proofs and additional information see §54 in
Paul R.. Halmos. *Finite-dimensional Vector Spaces*. Springer, New York, Heidelberg, Berlin, 1974

4.23.1 Definition

A scalar λ is a *proper value* or *eigenvalue*, and a non-zero vector $\mathbf{x}$ is a *proper vector* or *eigenvector* of a linear transformation A if

$$\mathsf{A}\mathbf{x} = \lambda \mathbf{x}. \tag{4.72}$$

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

4.23.2 Determination

Since the eigenvalues and eigenvectors are those scalars λ vectors $\mathbf{x}$ for which $\mathsf{A}\mathbf{x} = \lambda\mathbf{x}$, this equation can be rewritten with a zero vector on the right side of the equation; that is ($\mathsf{I} = \text{diag}(1, \ldots, 1)$ stands for the identity matrix),

$$(\mathsf{A} - \lambda \mathsf{I})\mathbf{x} = \mathbf{0}. \tag{4.73}$$

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

We are not interested in this trivial solution of Eq. (4.73). Therefore, suppose that, contrary to the previous assumption, $\mathsf{A} - \lambda\mathsf{I}$ is *not* invertible. We have mentioned earlier (without proof) that this implies that its determinant vanishes; that is,

$$\det(\mathsf{A} - \lambda\mathsf{I}) = |\mathsf{A} - \lambda\mathsf{I}| = 0. \tag{4.74}$$

This is called the *sekular determinant*; and the corresponding equation after expansion of the determinant is called the *sekular 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. (4.73).

For the sake of an example, consider the matrix

$$A = \begin{pmatrix} 1 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 1 \end{pmatrix}. \tag{4.75}$$

The secular determinant yields

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

which yields 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 $\lambda(1-\lambda)(2-\lambda) = 0$.

Let us now determine the eigenvectors of A, based on the eigenvalues. Insertion $\lambda_1 = 0$ into Eq. (4.73) yields

$$\left[\begin{pmatrix} 1 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 1 \end{pmatrix} - \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}\right]\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 1 \end{pmatrix}\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}; \tag{4.76}$$

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. (4.73) yields

$$\left[\begin{pmatrix} 1 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 1 \end{pmatrix} - \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}\right]\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}; \tag{4.77}$$

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. (4.73) yields

$$\left[\begin{pmatrix} 1 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 1 \end{pmatrix} - \begin{pmatrix} 2 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{pmatrix}\right]\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} -1 & 0 & 1 \\ 0 & -1 & 0 \\ 1 & 0 & -1 \end{pmatrix}\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}; \tag{4.78}$$

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

Note that the eigenvectors are mutually orthogonal. We can construct the corresponding orthogonal projectors by the dyadic product of the eigenvectors; that is,

$$\begin{aligned}
\mathbf{E}_1 = \mathbf{x}_1 \otimes \mathbf{x}_1^T = \frac{1}{2}(1,0,-1)^T(1,0,-1) = \frac{1}{2}\begin{pmatrix} 1(1,0,-1) \\ 0(1,0,-1) \\ -1(1,0,-1) \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1 & 0 & -1 \\ 0 & 0 & 0 \\ -1 & 0 & 1 \end{pmatrix} \\
\mathbf{E}_2 = \mathbf{x}_2 \otimes \mathbf{x}_2^T = (0,1,0)^T(0,1,0) = \begin{pmatrix} 0(0,1,0) \\ 1(0,1,0) \\ 0(0,1,0) \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \\
\mathbf{E}_3 = \mathbf{x}_3 \otimes \mathbf{x}_3^T = \frac{1}{2}(1,0,1)^T(1,0,1) = \frac{1}{2}\begin{pmatrix} 1(1,0,1) \\ 0(1,0,1) \\ 1(1,0,1) \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 1 \end{pmatrix}
\end{aligned} \tag{4.79}$$

Note also that A can be written as the sum of the products of the eigenvalues with the associated projectors; that is (here, $\mathbf{E}$ stands for the corresponding matrix), $A = 0\mathbf{E}_1 + 1\mathbf{E}_2 + 2\mathbf{E}_3$.

If the eigenvalues obtained are not distinct und 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

$$B = \begin{pmatrix} 1 & 0 & 1 \\ 0 & 2 & 0 \\ 1 & 0 & 1 \end{pmatrix}. \tag{4.80}$$

The secular determinant 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. (4.73) yields

$$\left[\begin{pmatrix} 1 & 0 & 1 \\ 0 & 2 & 0 \\ 1 & 0 & 1 \end{pmatrix} - \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}\right]\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 1 \\ 0 & 2 & 0 \\ 1 & 0 & 1 \end{pmatrix}\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}; \tag{4.81}$$

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. (4.73) yields

$$\left[\begin{pmatrix} 1 & 0 & 1 \\ 0 & 2 & 0 \\ 1 & 0 & 1 \end{pmatrix} - \begin{pmatrix} 2 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{pmatrix}\right] \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} -1 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & -1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}; \tag{4.82}$$

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 $x_1 = x_3$ 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 projectors by the dyadic product of the eigenvectors; that is, by

$$\begin{aligned}
\mathbf{E}_1 = \mathbf{x}_1 \otimes \mathbf{x}_1^T = \tfrac{1}{2}(1,0,-1)^T(1,0,-1) = \tfrac{1}{2}\begin{pmatrix} 1(1,0,-1) \\ 0(1,0,-1) \\ -1(1,0,-1) \end{pmatrix} = \tfrac{1}{2}\begin{pmatrix} 1 & 0 & -1 \\ 0 & 0 & 0 \\ -1 & 0 & 1 \end{pmatrix} \\
\mathbf{E}_{2,1} = \mathbf{x}_{2,1} \otimes \mathbf{x}_{2,1}^T = (0,1,0)^T(0,1,0) = \begin{pmatrix} 0(0,1,0) \\ 1(0,1,0) \\ 0(0,1,0) \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \\
\mathbf{E}_{2,2} = \mathbf{x}_{2,2} \otimes \mathbf{x}_{2,2}^T = \tfrac{1}{2}(1,0,1)^T(1,0,1) = \tfrac{1}{2}\begin{pmatrix} 1(1,0,1) \\ 0(1,0,1) \\ 1(1,0,1) \end{pmatrix} = \tfrac{1}{2}\begin{pmatrix} 1 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 1 \end{pmatrix}
\end{aligned} \tag{4.83}$$

Note also that B can be written as the sum of the products of the eigenvalues with the associated projectors; that is (here, $\mathbf{E}$ stands for the corresponding matrix), $B = 0\mathbf{E}_1 + 2(\mathbf{E}_{1,2} + \mathbf{E}_{1,2})$. This leads us to the much more general spectral theorem.

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 stricly positive, then every proper value of $\mathbf{A}$ is positive, or stricly positive, respectively

Due to their idempotence $\mathbf{EE} = \mathbf{E}$, projectors 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.

4.24 Normal transformation

A transformation $\mathbf{A}$ is called *normal* if it commutes with its adjoint; that is, $[\mathbf{A}, \mathbf{A}^*] = \mathbf{AA}^* - \mathbf{A}^*\mathbf{A} = 0$.

It follows from their definition that Hermitean and unitary transformations are normal.

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.

4.25 *Spectrum*

4.25.1 *Spectral theorem*

For proofs and additional information see §78 in

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

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

(i) the λ_i are pairwise distinct,

(ii) the E_i are pairwise orthogonal and different from $\mathbf{0}$,

(iii) $\sum_{i=1}^{k} \mathsf{E}_i = \mathsf{I}_n$, and

(iv) $\mathsf{A} = \sum_{i=1}^{k} \lambda_i \mathsf{E}_i$ is the *spectral form* of A.

4.25.2 *Composition of the spectral form*

If the spectrum of a Hermitian (or, more general, normal) operator A is nondegenerate, that is, $k = n$, then the ith projector can be written as the dyadic or tensor product $\mathsf{E}_i = \mathbf{x}_i \otimes \mathbf{x}_i^T$ of the ith normalized eigenvector $\mathbf{x}_i$ of A. In this case, the set of all normalized eigenvectors $\{\mathbf{x}_1, \ldots, \mathbf{x}_n\}$ is n othonormal basis of the vector space $\mathfrak{V}$. If the spectrum of A is degenerate, then the projector can be chosen to be the orthogonal sum of projectors corresponding to orthogonal eigenvectors, associated with the same eigenvalues.

Furthermore, for a Hermitian (or, more general, normal) operator A, if $1 \le i \le k$, then there exist polynomials with real coefficients, such as, for instance,

$$p_i(t) = \prod_{\substack{1 \le j \le k \\ j \ne i}} \frac{t - \lambda_j}{\lambda_i - \lambda_j} \tag{4.84}$$

so that $p_i(\lambda_j) = \delta_{ij}$; moreover, for every such polynomial, $p_i(\mathsf{A}) = \mathsf{E}_i$.

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 $j \ne i$, since some numerator in the product of fractions vanishes.

Now, substituting for t the spectral form $\mathsf{A} = \sum_{i=1}^{k} \lambda_i \mathsf{E}_i$ of A, as well as decomposing unity in terms of the projectors E_i in the spectral form of A;

that is, $\mathbf{I}_n = \sum_{i=1}^k \mathbf{E}_i$, yields

$$\begin{aligned} p_i(\mathbf{A}) &= \prod_{1\le j\le k,\, j\ne i} \frac{\mathbf{A}-\lambda_j \mathbf{I}_n}{\lambda_i-\lambda_j} \\ &= \prod_{1\le j\le k,\, j\ne i} \frac{\sum_{l=1}^k \lambda_l \mathbf{E}_l - \lambda_j \sum_{l=1}^k \mathbf{E}_l}{\lambda_i-\lambda_j} \\ &= \prod_{1\le j\le k,\, j\ne i} \frac{\sum_{l=1}^k \mathbf{E}_l(\lambda_l-\lambda_j)}{\lambda_i-\lambda_j} \\ &= \sum_{l=1}^k \mathbf{E}_l \prod_{1\le j\le k,\, j\ne i} \frac{\lambda_l-\lambda_j}{\lambda_i-\lambda_j} \\ &= \sum_{l=1}^k \mathbf{E}_l \delta_{li} = \mathbf{E}_i. \end{aligned} \tag{4.85}$$

With the help of the polynomial $p_i(t)$ defined in Eq. (4.84), which requires knowledge of the eigenvalues, the spectral form of a Hermitian (or, more general, normal) operator $\mathbf{A}$ can thus be rewritten as

$$\mathbf{A} = \sum_{i=1}^k \lambda_i p_i(\mathbf{A}) = \sum_{i=1}^k \lambda_i \prod_{1\le j\le k,\, j\ne i} \frac{\mathbf{A}-\lambda_j \mathbf{I}_n}{\lambda_i-\lambda_j}. \tag{4.86}$$

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 commuts with each $\mathbf{E}_i$, $1 \le i \le r$.

4.26 Functions of normal transformations

Suppose $\mathbf{A} = \sum_{i=1}^k \lambda_i \mathbf{E}_i$ is a normal transformation with 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

$$f(\mathbf{A}) = \sum_{i=1}^k f(\lambda_i)\mathbf{E}_i. \tag{4.87}$$

For the definition of the "square root" for every positve operator $\mathbf{A}$), consider

$$\sqrt{\mathbf{A}} = \sum_{i=1}^k \sqrt{\lambda_i}\mathbf{E}_i. \tag{4.88}$$

Clearly, $(\sqrt{\mathbf{A}})^2 = \sqrt{\mathbf{A}}\sqrt{\mathbf{A}} = \mathbf{A}$.

4.27 Decomposition of operators

4.27.1 Standard decomposition

For proofs and additional information see §83 in
Paul R.. Halmos. *Finite-dimensional Vector Spaces*. Springer, New York, Heidelberg, Berlin, 1974

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 $\mathbf{A}$ on a finite-dimensional vector space can be decomposed into two Hermitian operators $\mathbf{B}$ $\mathbf{C}$ such that

$$\begin{aligned} &\mathbf{A} = \mathbf{B} + i\mathbf{C}; \text{ with} \\ &\mathbf{B} = \tfrac{1}{2}(\mathbf{A}+\mathbf{A}^\dagger), \\ &\mathbf{C} = \tfrac{1}{2i}(\mathbf{A}-\mathbf{A}^\dagger). \end{aligned} \tag{4.89}$$

4.27.2 *Polar representation*

The analogue of the polar representation of every imaginary number $z = Re^{i\varphi}$ with $R, \varphi \in \mathbb{R}$, $R > 0$, $0 \le \varphi < 2\pi$, 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 $\mathbf{A} = \mathbf{UP}$. 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 $\mathbf{UP} = \mathbf{PU}$.

4.27.3 *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. [12], Chapter 2).

It has been suggested to implement these group theoretic results by realizing interferometric analogues of any discrete unitary and hermitean operators in a unified and experimentally feasible way by “generalized beam splitters” [13].

4.27.4 *Singular value decomposition*

The *singular value decomposition* (SVD) of an $(m \times n)$ matrix $\mathbf{A}$ is a factorization of the form

$$\mathbf{A} = \mathbf{U}\Sigma\mathbf{V}, \tag{4.90}$$

where $\mathbf{U}$ is a unitary $(m \times m)$ matrix (i.e. an isometry), $\mathbf{V}$ is a unitary $(n \times n)$ matrix, and Σ is a unique $(m \times n)$ diagonal matrix with nonnegative real numbers on the diagonal; that is,

$$\Sigma = \left(\begin{array}{ccc|ccc} \sigma_1 & & & & \vdots & \\ & \ddots & & \cdots & 0 & \cdots \\ & & \sigma_r & & \vdots & \\ \hline & \vdots & & & \vdots & \\ \cdots & 0 & \cdots & \cdots & 0 & \cdots \\ & \vdots & & & \vdots & \\ & \vdots & & & \vdots & \end{array}\right). \tag{4.91}$$

The entries $\sigma_1 \ge \sigma_2 \cdots \ge \sigma_r > 0$ of Σ are called *singular values* of $\mathbf{A}$. No proof is presented here.

[12] F. D. Murnaghan. *The Unitary and Rotation Groups*. Spartan Books, Washington, D.C., 1962

[13] 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

4.27.5 *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 $\{\mathbf{u}_1, \ldots, \mathbf{u}_n\} \subset \mathfrak{U}$ and $\{\mathbf{v}_1, \ldots, \mathbf{v}_m\} \subset \mathfrak{V}$ such that $\mathbf{z} = \sum_{i=1}^m \sigma_i \mathbf{u}_i \otimes \mathbf{v}_i$, where the σ_is are nonnegative scalars and the set of scalars is uniquely determined by $\mathbf{z}$.

Equivalently [14], 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 orthonoral vectors $|\mathbf{u}_i\rangle \in \mathfrak{U}$ and $|\mathbf{v}_j\rangle \in \mathfrak{V}$ so that

[14] M. A. Nielsen and I. L. Chuang. *Quantum Computation and Quantum Information*. Cambridge University Press, Cambridge, 2000

$$|\mathbf{z}\rangle = \sum_i \sigma_i |\mathbf{u}_i\rangle |\mathbf{v}_i\rangle, \tag{4.92}$$

where the σ_is are nonnegative scalars; if $|\mathbf{z}\rangle$ is normalized, then the σ_is 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 A. A can then be subjected to a singular value decomposition $\mathsf{A} = \mathsf{U}\Sigma\mathsf{V}$, or, written in index form (note that $\Sigma = \text{diag}(\sigma_1, \ldots, \sigma_n)$ 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 $|\mathbf{v}_l\rangle = \sum_l v_{lj} |j\rangle$ one obtains the Schmidt decompsition (4.92). Since u_{il} and v_{lj} represent unitary martices, 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 σ_is is one if $|\mathbf{z}\rangle$ is a unit vector, because (note that σ_is are real-valued) $\langle \mathbf{z}|\mathbf{z}\rangle = 1 = \sum_{lm} \sigma_l \sigma_m \langle \mathbf{u}_l|\mathbf{u}_m\rangle \langle \mathbf{v}_l|\mathbf{v}_m\rangle = \sum_{lm} \sigma_l \sigma_m \delta_{lm} = \sum_l \sigma_l^2$.

4.28 *Commutativity*

For proofs and additional information see §84 in Paul R.. Halmos. *Finite-dimensional Vector Spaces*. Springer, New York, Heidelberg, Berlin, 1974

A set $\mathsf{M} = \{\mathsf{A}_1, \mathsf{A}_2, \ldots, \mathsf{A}_k\}$ of self-adjoint transformations on a finite-dimensional inner product space are mutually commuting if and only if there exists a self-adjoint transformation R and a set of real-valued functions $F = \{f_1, f_2, \ldots, f_k\}$ of a real variable so that $\mathsf{A}_1 = f_1(\mathsf{R})$, $\mathsf{A}_2 = f_2(\mathsf{R})$, ..., $\mathsf{A}_k = f_k(\mathsf{R})$. If such a *maximal operator* R exists, then it can be written as a function of all transformations in the set M; that is, $\mathsf{R} = G(\mathsf{A}_1, \mathsf{A}_2, \ldots, \mathsf{A}_k)$, where G is a suitable real-valued function of n variables (cf. Ref. [15], Satz 8).

[15] John von Neumann. Über Funktionen von Funktionaloperatoren. *Annals of Mathematics*, 32:191–226, 1931. URL http://www.jstor.org/stable/1968185

The maximal operator R can be interpreted as containing all the information of a collection of commuting operators at once; stated pointedly, rather than consider all the operators in M separately, the maximal operator R represents M; in a sense, the operators $\mathsf{A}_i \in \mathsf{M}$ are all just incomplete *aspects* of, or individual functional views on, the maximal operator 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

$$\begin{aligned}
&\{\{1,-1,0\},\{(1,1,0)^T,(-1,1,0)^T,(0,0,1)^T\}\},\\
&\{\{5,-1,0\},\{(1,1,0)^T,(-1,1,0)^T,(0,0,1)^T\}\},\\
&\{\{12,-2,11\},\{(1,1,0)^T,(-1,1,0)^T,(0,0,1)^T\}\}.
\end{aligned}$$

They share a common orthonormal set of eigenvalues

$$\left\{ \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}, \frac{1}{\sqrt{2}}\begin{pmatrix} -1 \\ 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \right\}$$

which form an orthonormal basis of $\mathbb{R}^3$ or $\mathbb{C}^3$. The associated projectors are obtained by the dyadic or tensor products of these vectors; that is,

$$\begin{aligned}
\mathbf{E}_1 &= \tfrac{1}{2}\begin{pmatrix} 1 & 1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix},\\
\mathbf{E}_2 &= \tfrac{1}{2}\begin{pmatrix} 1 & -1 & 0 \\ -1 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix},\\
\mathbf{E}_3 &= \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}.
\end{aligned}$$

Thus the spectral decompositions of $\mathbf{A}$, $\mathbf{B}$ and $\mathbf{C}$ are

$$\begin{aligned}
\mathbf{A} &= \mathbf{E}_1 - \mathbf{E}_2 + 0\mathbf{E}_3,\\
\mathbf{B} &= 5\mathbf{E}_1 - \mathbf{E}_2 + 0\mathbf{E}_3,\\
\mathbf{C} &= 12\mathbf{E}_1 - 2\mathbf{E}_2 + 11\mathbf{E}_3,
\end{aligned} \tag{4.93}$$

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 projector coefficients obtained in Eq. (4.93); that is,

$$\begin{aligned}
\mathbf{A} &= f_{\mathbf{A}}(\mathbf{R}) = \mathbf{E}_1 - \mathbf{E}_2 + 0\mathbf{E}_3,\\
\mathbf{B} &= f_{\mathbf{B}}(\mathbf{R}) = 5\mathbf{E}_1 - \mathbf{E}_2 + 0\mathbf{E}_3,\\
\mathbf{C} &= f_{\mathbf{C}}(\mathbf{R}) = 12\mathbf{E}_1 - 2\mathbf{E}_2 + 11\mathbf{E}_3.
\end{aligned}$$

It is no coincidence that the projectors 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 projectors.

Let the set $\mathbf{M} = \{\mathbf{A}_1, \mathbf{A}_2, \ldots, \mathbf{A}_k\}$ be mutually commuting normal (or Hermitian, or self-adjoint) transformations on an n-dimensional inner product space. Then there exists an orthonormal basis $\mathfrak{B} = \{\mathbf{f}_1, \ldots, \mathbf{f}_n\}$ such that every $\mathbf{f}_j \in \mathfrak{B}$ is an eigenvalue of each of the $\mathbf{A}_i \in \mathbf{M}$. Equivalently, there exist n orthogonal projectors (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 $\mathbf{E}_j$, $1 \le j \le n$ occurs in the spectral form of each of the $\mathbf{A}_i \in \mathbf{M}$.

4.29 *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 projectors.

Suppose $\mathbf{E} = \{\mathbf{E}_1, \mathbf{E}_2, \ldots, \mathbf{E}_n\}$ is a set of mutually commuting orthogonal projectors on a finite-dimensional inner product space $\mathfrak{V}$. Then, the probability measure w should be *additive*; that is,

$$w(\mathbf{E}_1 + \mathbf{E}_2 \cdots + \mathbf{E}_n) = w(\mathbf{E}_1) + w(\mathbf{E}_2) + \cdots + w(\mathbf{E}_n). \tag{4.94}$$

Stated differently, we shall assume that, for any two orthogonal projectors $\mathbf{E}, \mathbf{F}$ so that $\mathbf{EF} = \mathbf{FE} = 0$, their sum $\mathbf{G} = \mathbf{E} + \mathbf{F}$ has expectation value

$$\langle \mathbf{G} \rangle = \langle \mathbf{E} \rangle + \langle \mathbf{F} \rangle. \tag{4.95}$$

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.

4.29.1 *Gleason's theorem*

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 [16]

$$\langle \mathbf{A} \rangle = \mathrm{Tr}(\rho \mathbf{A}), \tag{4.96}$$

the trace of the operator product of the density matrix (which is a positive operator of the trace class) ρ for the system with the matrix representation of $\mathbf{A}$.

In particular, if $\mathbf{A}$ is a projector $\mathbf{E}$ corresponding to an elementary yes-no proposition *"the system has property Q,"* then $\langle \mathbf{E} \rangle = \mathrm{Tr}(\rho \mathbf{E})$ corresponds to the probability of that property Q if the system is in state ρ.

[16] 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*, 162:287–312, 1999. DOI: 10.1006/jfan.1998.3372. URL http://dx.doi.org/10.1006/jfan.1998.3372; and Asher Peres. *Quantum Theory: Concepts and Methods*. Kluwer

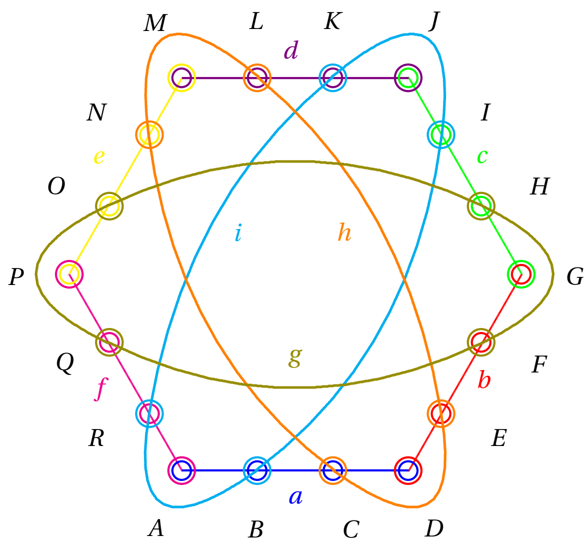
4.29.2 Kochen-Specker theorem

For a Hilbert space of dimension three or greater, there does not exist any two-valued probability measures interpretable as consistent, overall truth assignment [17]. 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.

[17] 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

In *Greechie diagram* [18], points represent basis vectors. If they belong to the same basis, they are connected by smooth curves.

[18] 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



The most compact way of deriving the Kochen-Specker theorem in four dimensions has been given by Cabello [19]. 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 projectors 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.

[19] 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; 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.

4.30 Hilbert space quantum mechanics and quantum logic

4.30.1 Quantum mechanics

The following is a very brief introduction to quantum mechanics. Introductions to quantum mechanics can be found in Refs. [20].

All quantum mechanical entities are represented by objects of Hilbert spaces [21]. 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 $\mathfrak{B} = \{\mathbf{b}_1, \mathbf{b}_2, \ldots, \mathbf{b}_n\}$ 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 δ_{ij} is the Kronecker delta function.

(I) A quantum *state* is represented by a positive Hermitian operator ρ 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 $i = 1, \ldots, n$, $\mathbf{b}_i \in \mathfrak{B}$, and $\sum_{i=1}^n p_i = 1$, so that

(ii) $\langle \rho\mathbf{x} \mid \mathbf{x}\rangle = \langle \mathbf{x} \mid \rho\mathbf{x}\rangle \geq 0$,

(iii) $\text{Tr}(\rho) = \sum_{i=1}^n \langle \mathbf{b}_i \mid \rho \mid \mathbf{b}_i\rangle = 1$.

A *pure state* is represented by a (unit) vector $\mathbf{x}$, also denoted by $\mid \mathbf{x}\rangle$, 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 $\mathfrak{H}$ spannned by the vector $\mathbf{x}$. Equivalently, it is represented by the projector $\mathsf{E}_\mathbf{x} = \mid \mathbf{x}\rangle\langle\mathbf{x}\mid$ 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 *coherent superposition* of state $\mathbf{x}$ and $\mathbf{y}$. Coherent state superpositions between classically mutually exclusive (i.e. orthogonal) states, say $\mid \mathbf{0}\rangle$ and $\mid \mathbf{1}\rangle$, 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 $\{\mathbf{b}_1, \mathbf{b}_2, \cdots \mathbf{b}_n\}$, that is, $\mathbf{x} = \sum_{i=1}^n \beta_i \mathbf{b}_i$, where n is

[20] 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

[21] John von Neumann. *Mathematische Grundlagen der Quantenmechanik*. Springer, Berlin, 1932; 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

the dimension of $\mathfrak{H}$ and $\beta_i = \langle \mathbf{b}_i \mid \mathbf{x}\rangle \in \mathbb{C}$.

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, synonymuously, Hermitian, operators or transformations $\mathsf{A} = \mathsf{A}^\dagger$ on the Hilbert space $\mathfrak{H}$ such that $\langle \mathsf{A}\mathbf{x} \mid \mathbf{y}\rangle = \langle \mathbf{x} \mid \mathsf{A}\mathbf{y}\rangle$ for all $\mathbf{x}, \mathbf{y} \in \mathfrak{H}$. (Observables and their corresponding operators are identified.)

The trace of an operator A is given by $\mathrm{Tr}\mathsf{A} = \sum_{i=1}^{n} \langle \mathbf{b}_i|\mathsf{A}|\mathbf{b}_i\rangle$.

Furthermore, any Hermitian operator has a spectral representation as a spectral sum $\mathsf{A} = \sum_{i=1}^{n} \alpha_i \mathsf{E}_i$, where the E_i's are orthogonal projection operators onto the orthonormal eigenvectors $\mathbf{a}_i$ of 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 A, B are compatible, if their *commutator* vanishes; that is, if $[\mathsf{A}, \mathsf{B}] = \mathsf{AB} - \mathsf{BA} = 0$.

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 [22].

(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 A. If $\mathbf{x}$ is in a coherent superposition of eigenstates of A, the particular outcome of any such single measurement is believed to be indeterministic [23]; 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 A with the associated real-valued eigenvalue α_i; that is, $\mathsf{A}\mathbf{x} = \alpha_n \mathbf{a}_n$ (no Einstein sum convention here).

This "transition" $\mathbf{x} \to \mathbf{a}_n$ 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 ψ-function? In his 1935 paper "Die Gegenwärtige Situation in der Quantenmechanik" ("The present situation in quantum mechanics" [24]), on page 53, Schrödinger states, *"the ψ-function as expectation-catalog:* … In it [[the ψ-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 ψ-function (=the prediction catalog) a characteristic, quite sudden

[22] 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

[23] 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

[24] 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

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 ψ-function has nothing whatever in common with its orderly development *between* two measurements. The abrupt change [[of the ψ-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 ψ-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. [25], 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."

German original: *"Die ψ-Funktion als Katalog der Erwartung:* … Sie [[die ψ-Funktion]] ist jetzt das Instrument zur Voraussage der Wahrscheinlichkeit von Maßzahlen. In ihr ist die jeweils erreichte Summe theoretisch begründeter Zukunftserwartung verkörpert, gleichsam wie in einem *Katalog* niedergelegt. … Bei jeder Messung ist man genötigt, der ψ-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 ψ-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 ψ-Funktion *nicht* direkt an die Stelle des Modells oder des Realdings setzen. Und zwar nicht etwa weil man einem Realding 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.

[25] Erwin Schrödinger. *The Interpretation of Quantum Mechanics. Dublin Seminars (1949-1955) and Other Unpublished Essays.* Ox Bow Press, Woodbridge, Connecticut, 1995

(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: $P_{\mathbf{x}}(\mathbf{y}) = \text{Tr}(\rho_{\mathbf{x}}\mathsf{E}_{\mathbf{y}})$. 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 $\rho_{\mathbf{x}} = \mathsf{E}_{\mathbf{x}} = |\mathbf{x}\rangle\langle\mathbf{x}|$ onto the unit vector $\mathbf{x}$; thus expansion of the trace and $\mathsf{E}_{\mathbf{y}} = |\mathbf{y}\rangle\langle\mathbf{y}|$ yields $P_{\mathbf{x}}(\mathbf{y}) = \sum_{i=1}^n \langle i \mid \mathbf{x}\rangle\langle\mathbf{x}|\mathbf{y}\rangle\langle\mathbf{y} \mid i\rangle = \sum_{i=1}^n \langle\mathbf{y} \mid i\rangle\langle i \mid \mathbf{x}\rangle\langle\mathbf{x}|\mathbf{y}\rangle = \sum_{i=1}^n \langle\mathbf{y} \mid \mathbf{1} \mid \mathbf{x}\rangle\langle\mathbf{x}|\mathbf{y}\rangle = |\langle\mathbf{y} \mid \mathbf{x}\rangle|^2$.

(V) The *average value* or *expectation value* of an observable A in a quantum state $\mathbf{x}$ is given by $\langle A\rangle_{\mathbf{y}} = \text{Tr}(\rho_{\mathbf{x}}\mathsf{A})$.

The *average value* or *expectation value* of an observable $\mathsf{A} = \sum_{i=1}^n \alpha_i \mathsf{E}_i$ in a pure state $\mathbf{x}$ is given by $\langle A\rangle_{\mathbf{x}} = \sum_{j=1}^n \sum_{i=1}^n \alpha_i \langle j \mid \mathbf{x}\rangle\langle\mathbf{x}|\mathbf{a}_i\rangle\langle\mathbf{a}_i \mid j\rangle = \sum_{j=1}^n \sum_{i=1}^n \alpha_i \langle\mathbf{a}_i \mid j\rangle\langle j \mid \mathbf{x}\rangle\langle\mathbf{x}|\mathbf{a}_i\rangle = \sum_{j=1}^n \sum_{i=1}^n \alpha_i \langle\mathbf{a}_i \mid \mathbf{1} \mid \mathbf{x}\rangle\langle\mathbf{x}|\mathbf{a}_i\rangle = \sum_{i=1}^n \alpha_i |\langle\mathbf{x} \mid \mathbf{a}_i\rangle|^2$.

(VI) The dynamical law or equation of motion can be written in the form $x(t) = \mathsf{U}x(t_0)$, where $\mathsf{U}^\dagger = \mathsf{U}^{-1}$ ("† 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 ψ_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, [26] for a detailed treatment of various Hamiltonians $\mathbf{H}$.)

[26] A. S. Davydov. *Quantum Mechanics.* Addison-Wesley, Reading, MA, 1965

4.30.2 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 4.1 lists the identifications of relations of operations of classical Boolean set-theoretic and quantum Hillbert 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	$\mathbf{E}_1\mathbf{E}_2 = \mathbf{E}_1$	$\mathbf{E}_1\mathbf{E}_2$ $\{\lim_{n\to\infty}(\mathbf{E}_1\mathbf{E}_2)^n\}$	$\mathbf{E}_1 + \mathbf{E}_2 - \mathbf{E}_1\mathbf{E}_2$	orthogonal projection

Table 4.1: 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 $\mathbf{E_p}$ (recall that $\mathbf{E_p}\mathbf{E_p} = \mathbf{E_p}$).

(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 $\mathfrak{M}_\mathbf{q}$,

$$\mathfrak{M}_{\mathbf{p}\wedge q} = \{x \mid x \in \mathfrak{M}_\mathbf{p},\ x \in \mathfrak{M}_\mathbf{q}\}.$$

(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 q and their associated closed linear subspaces $\mathfrak{M}_\mathbf{p}$ and $\mathfrak{M}_\mathbf{q}$,

$$\mathfrak{M}_{\mathbf{p}\vee q} = \mathfrak{M}_\mathbf{p} \oplus \mathfrak{M}_\mathbf{q} = \{\mathbf{x} \mid \mathbf{x} = \alpha\mathbf{y} + \beta\mathbf{z},\ \alpha,\beta \in \mathbb{C},\ \mathbf{y} \in \mathfrak{M}_\mathbf{p},\ \mathbf{z} \in \mathfrak{M}_\mathbf{q}\}.$$

The symbol $\oplus$ will 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 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 $\mathfrak{M}_\mathbf{q}$,

$$p \rightarrow q \Longleftrightarrow \mathfrak{M}_\mathbf{p} \subset \mathfrak{M}_\mathbf{q}.$$

(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,

$$\mathfrak{M}_0 = 0.$$

4.30.3 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* [27]. 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 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 [28] utilizing a configuration sketched in Fig. 4.5 claim to be able to infer two different contexts

[27] 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

[28] 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

counterfactually. One context is measured on one side of the setup, the other context on the other side of it. By the uniqueness property [29] 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.

[29] Karl Svozil. Are simultaneous Bell measurements possible? *New Journal of Physics*, 8:39, 1–8, 2006. DOI: 10.1088/1367-2630/8/3/039. URL http://dx.doi.org/10.1088/1367-2630/8/3/039

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.

4.30.4 *Realizations of two-dimensional beam splitters*

In what follows, lossless devices will be considered. The matrix

$$\mathbf{T}(\omega,\phi)=\begin{pmatrix}\sin\omega & \cos\omega\\ e^{-i\phi}\cos\omega & -e^{-i\phi}\sin\omega\end{pmatrix} \tag{4.97}$$

introduced in Eq. (4.97) 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. 4.2. The elementary quantum interference device $\mathbf{T}^{bs}$ in Fig. 4.2a) 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 [30]

[30] 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

$$\begin{array}{rcll}P_1: & |\mathbf{0}\rangle & \rightarrow & |\mathbf{0}\rangle e^{i(\alpha+\beta)},\\ P_2: & |\mathbf{1}\rangle & \rightarrow & |\mathbf{1}\rangle e^{i\beta},\\ S: & |\mathbf{0}\rangle & \rightarrow & \sqrt{T}\,|\mathbf{1}'\rangle+i\sqrt{R}\,|\mathbf{0}'\rangle,\\ S: & |\mathbf{1}\rangle & \rightarrow & \sqrt{T}\,|\mathbf{0}'\rangle+i\sqrt{R}\,|\mathbf{1}'\rangle,\\ P_3: & |\mathbf{0}'\rangle & \rightarrow & |\mathbf{0}'\rangle e^{i\varphi},\end{array} \tag{4.98}$$

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 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

$$\mathbf{T}^{bs}(\omega,\alpha,\beta,\varphi)=\begin{pmatrix}i\,e^{i\,(\alpha+\beta+\varphi)}\sin\omega & e^{i\,(\beta+\varphi)}\cos\omega\\ e^{i\,(\alpha+\beta)}\cos\omega & i\,e^{i\,\beta}\sin\omega\end{pmatrix}. \tag{4.99}$$

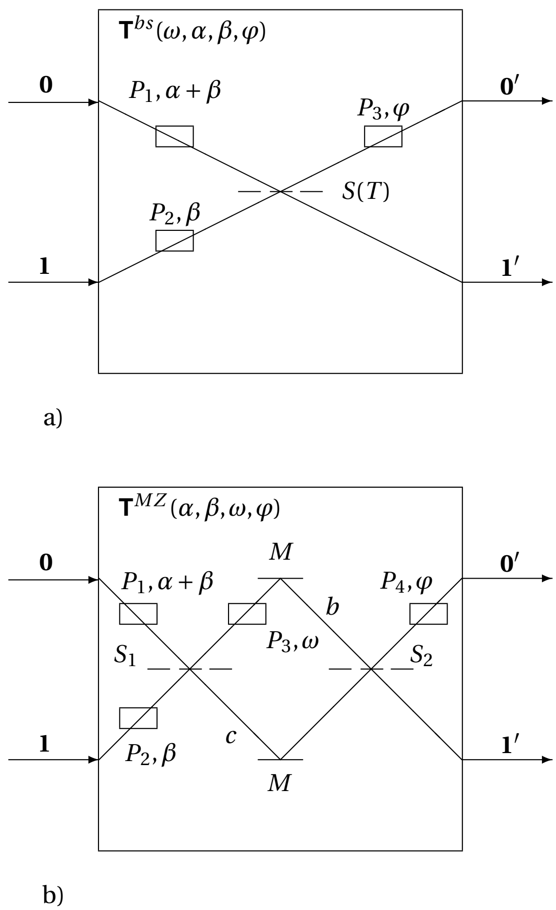


Figure 4.2: A universal quantum interference device operating on a qubit can be realized by a 4-port interferometer with two input ports **0**, **1** and two output ports **0**′, **1**′; a) realization by a single beam splitter $S(T)$ with variable transmission T and three phase shifters P_1, P_2, P_3; 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.

Alternatively, the action of a lossless beam splitter may be described by the matrix [31]

$$\begin{pmatrix} i\sqrt{R(\omega)} & \sqrt{T(\omega)} \\ \sqrt{T(\omega)} & i\sqrt{R(\omega)} \end{pmatrix} = \begin{pmatrix} i\sin\omega & \cos\omega \\ \cos\omega & i\sin\omega \end{pmatrix}.$$

A phase shifter in two-dimensional Hilbert space is represented by either $\text{diag}\left(e^{i\varphi},1\right)$ or $\text{diag}\left(1,e^{i\varphi}\right)$. 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 [32]; i.e.,

$$\mathbf{T}^{bs}(\omega,\alpha,\beta,\varphi) = \begin{pmatrix} e^{i\varphi} & 0 \\ 0 & 1 \end{pmatrix}\begin{pmatrix} i\sin\omega & \cos\omega \\ \cos\omega & i\sin\omega \end{pmatrix}\begin{pmatrix} e^{i(\alpha+\beta)} & 0 \\ 0 & 1 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & e^{i\beta} \end{pmatrix}. \tag{4.100}$$

The elementary quantum interference device $\mathbf{T}^{MZ}$ depicted in Fig. 4.2b) is a Mach-Zehnder interferometer with *two* input and output ports and three phase shifters. The process can be quantum mechanically described by

$$\begin{array}{llcl} P_1: & |\mathbf{0}\rangle & \rightarrow & |\mathbf{0}\rangle e^{i(\alpha+\beta)}, \\ P_2: & |\mathbf{1}\rangle & \rightarrow & |\mathbf{1}\rangle e^{i\beta}, \\ S_1: & |\mathbf{1}\rangle & \rightarrow & (|b\rangle + i\,|c\rangle)/\sqrt{2}, \\ S_1: & |\mathbf{0}\rangle & \rightarrow & (|c\rangle + i\,|b\rangle)/\sqrt{2}, \\ P_3: & |b\rangle & \rightarrow & |b\rangle e^{i\omega}, \\ S_2: & |b\rangle & \rightarrow & (|\mathbf{1}'\rangle + i\,|\mathbf{0}'\rangle)/\sqrt{2}, \\ S_2: & |c\rangle & \rightarrow & (|\mathbf{0}'\rangle + i\,|\mathbf{1}'\rangle)/\sqrt{2}, \\ P_4: & |\mathbf{0}'\rangle & \rightarrow & |\mathbf{0}'\rangle e^{i\varphi}. \end{array} \tag{4.101}$$

The corresponding unitary evolution matrix is given by

$$\mathbf{T}^{MZ}(\alpha,\beta,\omega,\varphi) = i\,e^{i\left(\beta+\frac{\omega}{2}\right)}\begin{pmatrix} -e^{i(\alpha+\varphi)}\sin\frac{\omega}{2} & e^{i\varphi}\cos\frac{\omega}{2} \\ e^{i\alpha}\cos\frac{\omega}{2} & \sin\frac{\omega}{2} \end{pmatrix}. \tag{4.102}$$

Alternatively, $\mathbf{T}^{MZ}$ can be computed by matrix multiplication; i.e.,

$$\begin{aligned} \mathbf{T}^{MZ}(\alpha,\beta,\omega,\varphi) = i\,e^{i\left(\beta+\frac{\omega}{2}\right)}&\begin{pmatrix} e^{i\varphi} & 0 \\ 0 & 1 \end{pmatrix}\frac{1}{\sqrt{2}}\begin{pmatrix} i & 1 \\ 1 & i \end{pmatrix}\begin{pmatrix} e^{i\omega} & 0 \\ 0 & 1 \end{pmatrix}\cdot \\ &\cdot\frac{1}{\sqrt{2}}\begin{pmatrix} i & 1 \\ 1 & i \end{pmatrix}\begin{pmatrix} e^{i(\alpha+\beta)} & 0 \\ 0 & 1 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & e^{i\beta} \end{pmatrix}. \end{aligned} \tag{4.103}$$

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 the elementary beam splitter $\mathbf{T}$ in Eq. (4.97), 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

$$\mathbf{T}(\omega,\phi) = \mathbf{T}^{bs}(\omega,-\frac{\pi}{2},\frac{\pi}{2}-\phi,\phi-\frac{\pi}{2}) = \mathbf{T}^{MZ}(2\omega,\pi,\frac{\pi}{2}-\omega-\phi,\phi-\pi). \tag{4.104}$$

[31] The standard labelling of the input and output ports are interchanged, therefore sine and cosine are exchanged in the transition matrix.

[32] 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 R. A. Campos, B. E. A. Saleh, and M. 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

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

$$\mathbb{I}_2 = \mathbf{T}(\frac{\pi}{2},\pi) = \mathbf{T}^{bs}(\frac{\pi}{2},-\frac{\pi}{2},-\frac{\pi}{2},\frac{\pi}{2}) = \mathbf{T}^{MZ}(\pi,\pi,-\pi,0) = \text{diag}(1,1) \quad . \tag{4.105}$$

The "$\texttt{not}$" gate is defined by $|\mathbf{0}\rangle \rightarrow |\mathbf{1}\rangle$, $|\mathbf{1}\rangle \rightarrow |\mathbf{0}\rangle$ and can be realized by

$$\texttt{not} = \mathbf{T}(0,0) = \mathbf{T}^{bs}(0,-\frac{\pi}{2},\frac{\pi}{2},-\frac{\pi}{2}) = \mathbf{T}^{MZ}(0,\pi,\frac{\pi}{2},\pi) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad . \tag{4.106}$$

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

$$\sqrt{\mathbb{I}_2} = \mathbf{T}(\frac{\pi}{4},0) = \mathbf{T}^{bs}(\frac{\pi}{4},-\frac{\pi}{2},\frac{\pi}{2},-\frac{\pi}{2}) = \mathbf{T}^{MZ}(\frac{\pi}{2},\pi,\frac{\pi}{4},-\pi) = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \quad . \tag{4.107}$$

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 $\sqrt{\texttt{not}}$, such as

$$\sqrt{\texttt{not}} = \mathbf{T}^{bs}(\frac{\pi}{4},-\pi,\frac{3\pi}{4},-\pi) = \frac{1}{2}\begin{pmatrix} 1+i & 1-i \\ 1-i & 1+i \end{pmatrix}, \tag{4.108}$$

with $\sqrt{\texttt{not}}\sqrt{\texttt{not}} = \texttt{not}$.

4.30.5 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. [33], page 1, Fig. 1, and Fig. 4.3, 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.

[33] 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

The Cartesian (x,y,z)–coordinates can be translated into spherical coordinates (r,θ,φ) via $x = r\sin\theta\cos\varphi$, $y = r\sin\theta\sin\varphi$, $z = r\cos\theta$, whereby θ is the polar angle in the x–z-plane measured from the z-axis, with $0 \leq \theta \leq \pi$, and φ 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 θ and φ, 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

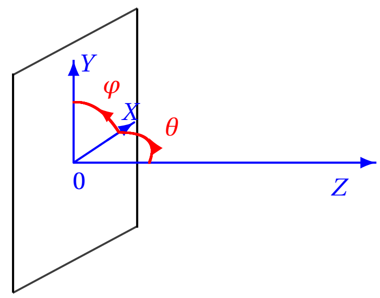


Figure 4.3: Coordinate system for measurements of particles travelling along $0Z$

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 ith experiment for a total of N experiments; i.e.,

$$E(a,b) = \frac{1}{N}\sum_{i=1}^{N} O(a)_i O(b)_i. \tag{4.109}$$

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"* [34], Chap. VI, Sec.24 in arbitrary directions, given by the spherical angular momentum co-ordinates θ and φ, 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 [35] quantum logic [36], 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.

[34] Leonard I. Schiff. *Quantum Mechanics*. McGraw-Hill, New York, 1955

[35] John von Neumann. *Mathematische Grundlagen der Quantenmechanik*. Springer, Berlin, 1932

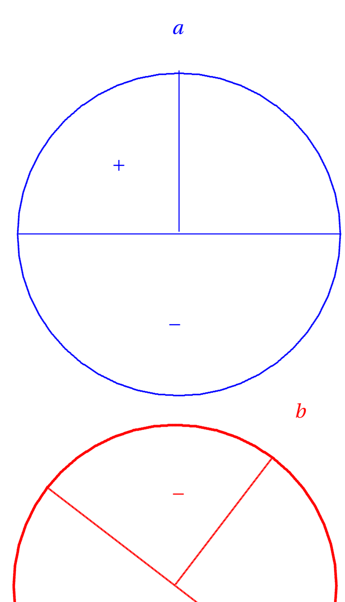
[36] Garrett Birkhoff and John von Neumann. The logic of quantum mechanics. *Annals of Mathematics*, 37(4):823–843, 1936. DOI: 10.2307/1968621. URL http://dx.doi.org/10.2307/1968621

Two-state particles:

Classical case:

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 $0X$ and $0Y$, as depicted in Figs. 4.3 and 4.4.

By considering the length $A_+(a,b)$ and $A_-(a,b)$ of the positive and



negative contributions to expectation function, one obtains for $0 \le \theta = |a-b| \le \pi$,

$$\begin{aligned} E_{\text{cl},2,2}(\theta) = E_{\text{cl},2,2}(a,b) &= \frac{1}{2\pi}\left[A_+(a,b) - A_-(a,b)\right] \\ &= \frac{1}{2\pi}\left[2A_+(a,b) - 2\pi\right] = \frac{2}{\pi}|a-b| - 1 = \frac{2\theta}{\pi} - 1, \end{aligned} \tag{4.110}$$

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 $\mathbf{a} = (a_1, a_2, \ldots, a_n)^T$ with respect to some basis of n-dimensional Hilbert space is obtained by taking the dyadic product; i.e., by

$$\mathbf{E_a} = \left[\mathbf{a}, \mathbf{a}^\dagger\right] = \left[\mathbf{a}, (\mathbf{a}^*)^T\right] = \mathbf{a}\otimes\mathbf{a}^\dagger = \begin{pmatrix} a_1\mathbf{a}^\dagger \\ a_2\mathbf{a}^\dagger \\ \cdots \\ a_n\mathbf{a}^\dagger \end{pmatrix} = \begin{pmatrix} a_1a_1^* & a_1a_2^* & \ldots & a_1a_n^* \\ a_2a_1^* & a_2a_2^* & \ldots & a_2a_n^* \\ \ldots & \ldots & \ldots & \ldots \\ a_na_1^* & a_na_2^* & \ldots & a_na_n^* \end{pmatrix}. \tag{4.111}$$

The tensor or Kronecker product of two vectors $\mathbf{a}$ and $\mathbf{b} = (b_1, b_2, \ldots, b_m)^T$ can be represented by

$$\mathbf{a}\otimes\mathbf{b} = (a_1\mathbf{b}, a_2\mathbf{b}, \ldots, a_n\mathbf{b})^T = (a_1b_1, a_1b_2, \ldots, a_nb_m)^T \tag{4.112}$$

The tensor or Kronecker product of some operators

$$\mathbf{A} = \begin{pmatrix} a_{11} & a_{12} & \ldots & a_{1n} \\ a_{21} & a_{22} & \ldots & a_{2n} \\ \ldots & \ldots & \ldots & \ldots \\ a_{n1} & a_{n2} & \ldots & a_{nn} \end{pmatrix} \text{ and } \mathbf{B} = \begin{pmatrix} b_{11} & b_{12} & \ldots & b_{1m} \\ b_{21} & b_{22} & \ldots & b_{2m} \\ \ldots & \ldots & \ldots & \ldots \\ b_{m1} & b_{m2} & \ldots & b_{mm} \end{pmatrix} \tag{4.113}$$

is represented by an $nm \times nm$-matrix

$$\mathbf{A}\otimes\mathbf{B} = \begin{pmatrix} a_{11}B & a_{12}B & \ldots & a_{1n}B \\ a_{21}B & a_{22}B & \ldots & a_{2n}B \\ \ldots & \ldots & \ldots & \ldots \\ a_{n1}B & a_{n2}B & \ldots & a_{nn}B \end{pmatrix} = \begin{pmatrix} a_{11}b_{11} & a_{11}b_{12} & \ldots & a_{1n}b_{1m} \\ a_{11}b_{21} & a_{11}b_{22} & \ldots & a_{2n}b_{2m} \\ \ldots & \ldots & \ldots & \ldots \\ a_{nn}b_{m1} & a_{nn}b_{m2} & \ldots & a_{nn}b_{mm} \end{pmatrix}. \tag{4.114}$$

Observables:

Let us start with the spin one-half angular momentum observables of *a single* particle along an arbitrary direction in spherical co-ordinates θ and φ in units of $\hbar$ [37]; i.e.,

[37] Leonard I. Schiff. *Quantum Mechanics*. McGraw-Hill, New York, 1955

$$\mathbf{M}_x = \frac{1}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \mathbf{M}_y = \frac{1}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \mathbf{M}_z = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (4.115)$$

The angular momentum operator in arbitrary direction θ, φ is given by its spectral decomposition

$$\begin{aligned}
\mathbf{S}_{\frac{1}{2}}(\theta,\varphi) &= x\mathbf{M}_x + y\mathbf{M}_y + z\mathbf{M}_z = \mathbf{M}_x \sin\theta\cos\varphi + \mathbf{M}_y \sin\theta\sin\varphi + \mathbf{M}_z\cos\theta \\
&= \tfrac{1}{2}\sigma(\theta,\varphi) = \tfrac{1}{2}\begin{pmatrix} \cos\theta & e^{-i\varphi}\sin\theta \\ e^{i\varphi}\sin\theta & -\cos\theta \end{pmatrix} \\
&= -\tfrac{1}{2}\begin{pmatrix} \sin^2\frac{\theta}{2} & -\frac{1}{2}e^{-i\varphi}\sin\theta \\ -\frac{1}{2}e^{i\varphi}\sin\theta & \cos^2\frac{\theta}{2} \end{pmatrix} + \tfrac{1}{2}\begin{pmatrix} \cos^2\frac{\theta}{2} & \frac{1}{2}e^{-i\varphi}\sin\theta \\ \frac{1}{2}e^{i\varphi}\sin\theta & \sin^2\frac{\theta}{2} \end{pmatrix} \\
&= -\tfrac{1}{2}\left\{\tfrac{1}{2}\left[\mathbb{I}_2 - \sigma(\theta,\varphi)\right]\right\} + \tfrac{1}{2}\left\{\tfrac{1}{2}\left[\mathbb{I}_2 + \sigma(\theta,\varphi)\right]\right\}.
\end{aligned} \quad (4.116)$$

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. (4.116) are

$$\begin{aligned}
|-\rangle_{\theta,\varphi} \equiv \mathbf{x}_{-\frac{1}{2}}(\theta,\varphi) &= e^{i\delta_+}\left(-e^{-\frac{i\varphi}{2}}\sin\tfrac{\theta}{2}, e^{\frac{i\varphi}{2}}\cos\tfrac{\theta}{2}\right), \\
|+\rangle_{\theta,\varphi} \equiv \mathbf{x}_{+\frac{1}{2}}(\theta,\varphi) &= e^{i\delta_-}\left(e^{-\frac{i\varphi}{2}}\cos\tfrac{\theta}{2}, e^{\frac{i\varphi}{2}}\sin\tfrac{\theta}{2}\right),
\end{aligned} \quad (4.117)$$

respectively. δ_+ and δ_- are arbitrary phases. These orthogonal unit vectors correspond to the two orthogonal projectors

$$\mathbf{F}_{\mp}(\theta,\varphi) = \frac{1}{2}\left[\mathbb{I}_2 \mp \sigma(\theta,\varphi)\right] \quad (4.118)$$

for the spin down and up states along θ and φ, 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. (4.120) can be rewritten to include all possible cases at once; i.e.,

$$\mathbf{S}_{\frac{1}{2}\frac{1}{2}}(\hat{\theta},\hat{\varphi}) = \mathbf{S}_{\frac{1}{2}}(\theta_1,\varphi_1) \otimes \mathbf{S}_{\frac{1}{2}}(\theta_2,\varphi_2). \quad (4.119)$$

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

$$\mathbf{F}_{\pm_1\pm_2}(\hat{\theta},\hat{\varphi}) = \frac{1}{2}\left[\mathbb{I}_2 \pm_1 \sigma(\theta_1,\varphi_1)\right] \otimes \frac{1}{2}\left[\mathbb{I}_2 \pm_2 \sigma(\theta_2,\varphi_2)\right]; \quad (4.120)$$

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. 4.5: $F_{-+}(\hat\theta,\hat\varphi)$ stands for the proposition

'The spin state of the first particle measured along θ_1, φ_1 is "$-$" and the spin state of the second particle measured along θ_2, φ_2 is "$+$".'

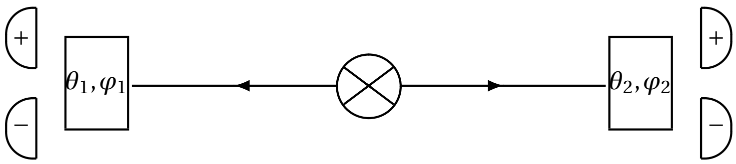


Figure 4.5: Simultaneous spin state measurement of the two-partite state represented in Eq. (4.123). Boxes indicate spin state analyzers such as Stern-Gerlach apparatus oriented along the directions θ_1, φ_1 and θ_2, φ_2; their two output ports are occupied with detectors associated with the outcomes "+" and "−", respectively.

More generally, we will consider two different numbers λ_+ and λ_-, and the generalized single-particle operator

$$\mathbf{R}_{\frac{1}{2}}(\theta,\varphi) = \lambda_- \left\{ \frac{1}{2}\left[\mathbb{I}_2 - \sigma(\theta,\varphi)\right]\right\} + \lambda_+ \left\{ \frac{1}{2}\left[\mathbb{I}_2 + \sigma(\theta,\varphi)\right]\right\}, \tag{4.121}$$

as well as the resulting two-particle operator

$$\begin{aligned} \mathbf{R}_{\frac{1}{2}\frac{1}{2}}(\hat\theta,\hat\varphi) &= \mathbf{R}_{\frac{1}{2}}(\theta_1,\varphi_1) \otimes \mathbf{R}_{\frac{1}{2}}(\theta_2,\varphi_2) \\ &= \lambda_-\lambda_- F_{--} + \lambda_-\lambda_+ F_{-+} + \lambda_+\lambda_- F_{+-} + \lambda_+\lambda_+ F_{++}. \end{aligned} \tag{4.122}$$

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 [38]. 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 $|\Psi^-\rangle$.

[38] 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

Consider the *singlet* "Bell" state of two spin-$\frac{1}{2}$ particles

$$|\Psi^-\rangle = \frac{1}{\sqrt{2}}\big(|+-\rangle - |-+\rangle\big). \tag{4.123}$$

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

$$\begin{aligned} |\Psi^-\rangle &\equiv \tfrac{1}{\sqrt{2}}(\mathbf{e}_1\otimes\mathbf{e}_2 - \mathbf{e}_2\otimes\mathbf{e}_1) \\ &= \tfrac{1}{\sqrt{2}}\left[(1,0)\otimes(0,1) - (0,1)\otimes(1,0)\right] = \left(0, \tfrac{1}{\sqrt{2}}, -\tfrac{1}{\sqrt{2}}, 0\right). \end{aligned} \tag{4.124}$$

The density operator ρ_{Ψ^-} is just the projector of the dyadic product of this vector, corresponding to the one-dimensional linear subspace spanned by

$|\Psi^-\rangle$; i.e.,

$$\rho_{\Psi^-} = |\Psi^-\rangle\langle\Psi^-| = \left[|\Psi^-\rangle, |\Psi^-\rangle^\dagger\right] = \frac{1}{2}\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & -1 & 0 \\ 0 & -1 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \tag{4.125}$$

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 θ, φ defined earlier [e. g., Ref. [39], Eq. (2), or Ref. [40], Eq. (7–49)].

[39] 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

[40] L. E. Ballentine. *Quantum Mechanics*. Prentice Hall, Englewood Cliffs, NJ, 1989

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 ρ_{Ψ^-} aligned or antialigned along the directions defined by (θ_1, φ_1) and (θ_2, φ_2) can be evaluated by a straightforward calculation of

$$\begin{aligned} P_{\Psi^-\pm_1\pm_2}(\hat\theta, \hat\varphi) &= \mathrm{Tr}\left[\rho_{\Psi^-}\cdot \mathbf{F}_{\pm_1\pm_2}(\hat\theta,\hat\varphi)\right] \\ &= \frac{1}{4}\left\{1 - (\pm_1 1)(\pm_2 1)\left[\cos\theta_1\cos\theta_2 + \sin\theta_1\sin\theta_2\cos(\varphi_1-\varphi_2)\right]\right\}. \end{aligned} \tag{4.126}$$

Again, "$\pm_i$," $i = 1,2$ refers to the outcome on the i'th particle.

Since $P_= + P_{\neq} = 1$ and $E = P_= - P_{\neq}$, 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 (θ_1, φ_1) and (θ_2, φ_2) are in terms of the expectation function given by

$$\begin{aligned} P_= = P_{++} + P_{--} &= \frac{1}{2}(1+E) \\ &= \frac{1}{2}\left\{1 - \left[\cos\theta_1\cos\theta_2 - \sin\theta_1\sin\theta_2\cos(\varphi_1-\varphi_2)\right]\right\}, \\ P_{\neq} = P_{+-} + P_{-+} &= \frac{1}{2}(1-E) \\ &= \frac{1}{2}\left\{1 + \left[\cos\theta_1\cos\theta_2 + \sin\theta_1\sin\theta_2\cos(\varphi_1-\varphi_2)\right]\right\}. \end{aligned} \tag{4.127}$$

Finally, the quantum mechanical expectation function is obtained by the difference $P_= - P_{\neq}$; i.e.,

$$E_{\Psi^- -1,+1}(\theta_1,\theta_2,\varphi_1,\varphi_2) = -\left[\cos\theta_1\cos\theta_2 + \cos(\varphi_1-\varphi_2)\sin\theta_1\sin\theta_2\right]. \tag{4.128}$$

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

$$\begin{aligned} E_{\Psi^- -1,+1}(\theta_1,\theta_2) &= -\cos(\theta_1 - \theta_2), \\ E_{\Psi^- -1,+1}(\tfrac{\pi}{2},\tfrac{\pi}{2},\varphi_1,\varphi_2) &= -\cos(\varphi_1 - \varphi_2). \end{aligned} \tag{4.129}$$

The general computation of the quantum expectation function for operator (4.122) yields

$$\begin{aligned} & E_{\Psi^- \lambda_1\lambda_2}(\hat{\theta},\hat{\varphi}) = \text{Tr}\left[\rho_{\Psi^-} \cdot R_{\frac{1}{2}\frac{1}{2}}\left(\hat{\theta},\hat{\varphi}\right)\right] = \\ & = \frac{1}{4}\left\{(\lambda_- + \lambda_+)^2 - (\lambda_- - \lambda_+)^2\left[\cos\theta_1\cos\theta_2 + \cos(\varphi_1-\varphi_2)\sin\theta_1\sin\theta_2\right]\right\}. \end{aligned} \tag{4.130}$$

The standard two-particle quantum mechanical expectations (4.128) 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 (4.119) 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.,

$$\begin{aligned} & E_{\Psi^- -\frac{1}{2},+\frac{1}{2}}(\hat{\theta},\hat{\varphi}) = \text{Tr}\left\{\rho_{\Psi^-} \cdot \left[S_{\frac{1}{2}}(\theta_1,\varphi_1) \otimes S_{\frac{1}{2}}(\theta_2,\varphi_2)\right]\right\} \\ & = \frac{1}{4}\left[\cos\theta_1\cos\theta_2 + \cos(\varphi_1-\varphi_2)\sin\theta_1\sin\theta_2\right] = \frac{1}{4}E_{\Psi^- -1,+1}(\hat{\theta},\hat{\varphi}). \end{aligned} \tag{4.131}$$

5
Tensors

What follows is a "corollary," or rather an extension, of what has been presented in the previous chapter; in particular, dual vector spaces (page 44), and the tensor product (page 48).

5.1 Notation

In what follows, let us consider the vector space $\mathbb{R}^n$ of dimension n; a basis $\mathfrak{B} = \{\mathbf{e}_1, \mathbf{e}_2, \ldots, \mathbf{e}_n\}$ consisting of n basis vectors $\mathbf{e}_i$, and k arbitrary vectors $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_k \in \mathbb{R}^n$; the vector $\mathbf{x}_i$ having the vector components $X_1^i, X_2^i, \ldots, X_k^i \in \mathbb{R}$ or $\mathbb{C}$.

Please note again that, just like any tensor (field), the tensor product $\mathbf{z} = \mathbf{x} \otimes \mathbf{y}$ 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 $\mathbf{z} = (X^1\mathbf{y}, X^2\mathbf{y}, \ldots, X^n\mathbf{y}) = (X^1Y^1, \ldots, X^1Y^n, \ldots, X^nY^1, \ldots, X^nY^n)$. Again, the scalar coordinates X^iY^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^iY^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 (one pair with a superscript and a subscript). Sometimes, sums are written out explicitly.

In what follows, the notations " $x \cdot y$", " (x,y)" and " $\langle x \mid y\rangle$" will be used synonymously for the *scalar product* or *inner product*. Note, however, that the notation " $x \cdot y$" may be a little bit misleading; for example, in the case of the "pseudo-Euclidean" metric $\text{diag}(+,+,+,\cdots,+,-)$ it is no more the standard Euclidean dot product $\text{diag}(+,+,+,\cdots,+,+)$.

For a more systematic treatment, see for instance Klingbeil's or Dirschmid's introductions [1].

[1] 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*

$$\alpha : \mathbb{R}^k \mapsto \mathbb{R} \tag{5.1}$$

is a map satisfying

$$\begin{aligned} \alpha(\mathbf{x}_1,\mathbf{x}_2,\ldots,A\mathbf{x}_i^1+B\mathbf{x}_i^2,\ldots,\mathbf{x}_k) \quad = \quad & A\alpha(\mathbf{x}_1,\mathbf{x}_2,\ldots,\mathbf{x}_i^1,\ldots,\mathbf{x}_k) \\ & +B\alpha(\mathbf{x}_1,\mathbf{x}_2,\ldots,\mathbf{x}_i^2,\ldots,\mathbf{x}_k) \end{aligned} \tag{5.2}$$

for every one of its (multi-)arguments.

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 tensor in an n–dimensional vector space $\mathfrak{V}$ labelled by an index i. A tensor of rank k

$$\alpha : \mathbb{R}^k \mapsto \mathbb{R} \tag{5.3}$$

is a multilinear form

$$\alpha(\mathbf{x}_1,\mathbf{x}_2,\ldots,\mathbf{x}_k) = \sum_{i_1=1}^n \sum_{i_2=1}^n \cdots \sum_{i_k=1}^n X_1^{i_1} X_2^{i_2} \ldots X_k^{i_k} \alpha(\mathbf{e}_{i_1},\mathbf{e}_{i_2},\ldots,\mathbf{e}_{i_k}). \tag{5.4}$$

The

$$A_{i_1 i_2 \cdots i_k} = \alpha(\mathbf{e}_{i_1},\mathbf{e}_{i_2},\ldots,\mathbf{e}_{i_k}) \tag{5.5}$$

are the *components* of the tensor α with respect to the basis $\mathfrak{B}$.

Question: how many coordinates are there?

Answer: n^k.

Question: proof that tensors are multilinear forms.

Answer: by insertion.

$$\alpha(\mathbf{x}_1,\mathbf{x}_2,\ldots,A\mathbf{x}_j^1+B\mathbf{x}_j^2,\ldots,\mathbf{x}_k)$$

$$
\begin{aligned}
&= \sum_{i_1=1}^{n}\sum_{i_2=1}^{n}\cdots\sum_{i_k=1}^{n} X_1^{i_i} X_2^{i_2}\dots[A(X^1)_j^{i_j}+B(X^2)_j^{i_j}]\dots X_k^{i_k}\alpha(\mathbf{e}_{i_1},\mathbf{e}_{i_2},\dots,\mathbf{e}_{i_j},\dots,\mathbf{e}_{i_k})\\
&= A\sum_{i_1=1}^{n}\sum_{i_2=1}^{n}\cdots\sum_{i_k=1}^{n} X_1^{i_i} X_2^{i_2}\dots(X^1)_j^{i_j}\dots X_k^{i_k}\alpha(\mathbf{e}_{i_1},\mathbf{e}_{i_2},\dots,\mathbf{e}_{i_j},\dots,\mathbf{e}_{i_k})\\
&\quad +B\sum_{i_1=1}^{n}\sum_{i_2=1}^{n}\cdots\sum_{i_k=1}^{n} X_1^{i_i} X_2^{i_2}\dots(X^2)_j^{i_j}\dots X_k^{i_k}\alpha(\mathbf{e}_{i_1},\mathbf{e}_{i_2},\dots,\mathbf{e}_{i_j},\dots,\mathbf{e}_{i_k})\\
&= A\alpha(\mathbf{x}_1,\mathbf{x}_2,\dots,\mathbf{x}_j^1,\dots,\mathbf{x}_k)+B\alpha(\mathbf{x}_1,\mathbf{x}_2,\dots,\mathbf{x}_j^2,\dots,\mathbf{x}_k)
\end{aligned}
$$

5.3.1 Basis transformations

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 $\mathfrak{B}$:

$$
\mathbf{e}'_i = \sum_{j=1}^{n} a_i^j \mathbf{e}_j, \qquad i = 1,\dots,n. \tag{5.6}
$$

Formally, one may treat $\mathbf{e}'_i$ and $\mathbf{e}_i$ as scalar variables e'_i and e_j, respectively; such that $a_i^j = \frac{\partial e'_i}{\partial e_j}$.

Consider an arbitrary vector $x \in \mathbb{R}^n$ with components X^i with respect to the basis $\mathfrak{B}$ and X'^i with respect to the basis $\mathfrak{B}'$:

$$
x = \sum_{i=1}^{n} X^i \mathbf{e}_i = \sum_{i=1}^{n} X'^i \mathbf{e}'_i. \tag{5.7}
$$

Insertion into (5.6) yields

$$
x = \sum_{i=1}^{n} X^i \mathbf{e}_i = \sum_{i=1}^{n} X'^i \mathbf{e}'_i = \sum_{i=1}^{n} X'^i \sum_{j=1}^{n} a_i^j \mathbf{e}_j = \sum_{i=1}^{n}\left[\sum_{j=1}^{n} a_i^j X'^i\right]\mathbf{e}_j. \tag{5.8}
$$

A comparison of coefficient yields the transformation laws of vector components

$$
X^j = \sum_{j=1}^{n} a_i^j X'^i. \tag{5.9}
$$

The matrix $a = \{a_i^j\}$ is called the *transformation matrix*. In terms of the coordinates X^j, it can be expressed as

$$
a_i^j = \frac{\partial X^j}{\partial X'_i}. \tag{5.10}
$$

A similar argument using

$$
\mathbf{e}_i = \sum_{j=1}^{n} a'^j_i \mathbf{e}'_j, \qquad i = 1,\dots,n \tag{5.11}
$$

yields the inverse transformation laws

$$
X'^j = \sum_{j=1}^{n} a'^j_i X^i. \tag{5.12}
$$

Again, formally, we may treat $\mathbf{e}'_i$ and $\mathbf{e}_i$ as scalar variables e'_i and e_j, respectively; such that $a'^{j}_{i} = \frac{\partial e_i}{\partial e'_j}$. Thereby,

$$\mathbf{e}_i = \sum_{j=1}^{n} a'^{j}_{i} \mathbf{e}'_j = \sum_{j=1}^{n} a'^{j}_{i} \sum_{k=1}^{n} a^{k}_{j} \mathbf{e}_k = \sum_{j=1}^{n} \sum_{k=1}^{n} [a'^{j}_{i} a^{k}_{j}] \mathbf{e}_k, \tag{5.13}$$

which, due to the linear independence of the basis vectors $\mathbf{e}_i$ of $\mathfrak{B}$, is only satisfied if

$$a'^{j}_{i} a^{k}_{j} = \delta^{k}_{i} \qquad \text{or} \qquad a' a = \mathbb{I}. \tag{5.14}$$

That is, a' is the inverse matrix of a. In terms of the coordinates X^j, it can be expressed as

$$a'^{j}_{i} = \frac{\partial X'^{j}}{\partial X_i}. \tag{5.15}$$

5.3.2 Transformation of Tensor components

Because of multilinearity (!) and by insertion into (5.6),

$$\begin{aligned} \alpha(\mathbf{e}'_{j_1}, \mathbf{e}'_{j_2}, \ldots, \mathbf{e}'_{j_k}) &= \alpha\left(\sum_{i_1=1}^{n} a^{i_1}_{j_1} \mathbf{e}_{i_1}, \sum_{i_2=1}^{n} a^{i_2}_{j_2} \mathbf{e}_{i_2}, \ldots, \sum_{i_k=1}^{n} a^{i_k}_{j_k} \mathbf{e}_{i_k} \right) \\ &= \sum_{i_1=1}^{n} \sum_{i_2=1}^{n} \cdots \sum_{i_k=1}^{n} a^{i_1}_{j_1} a^{i_2}_{j_2} \cdots a^{i_k}_{j_k} \alpha(\mathbf{e}_{i_1}, \mathbf{e}_{i_2}, \ldots, \mathbf{e}_{i_k}) \end{aligned} \tag{5.16}$$

or

$$A'_{j_1 j_2 \cdots j_k} = \sum_{i_1=1}^{n} \sum_{i_2=1}^{n} \cdots \sum_{i_k=1}^{n} a^{i_1}_{j_1} a^{i_2}_{j_2} \cdots a^{i_k}_{j_k} A_{i_1 i_2 \ldots i_k}. \tag{5.17}$$

5.4 Contravariant tensors

5.4.1 Definition of contravariant basis

Consider again a covariant basis $\mathfrak{B} = \{\mathbf{e}_1, \mathbf{e}_2, \ldots, \mathbf{e}_n\}$ consisting of n basis vectors $\mathbf{e}_i$. Just as on page 45 earlier, we shall define a *contravariant* basis $\mathfrak{B}^* = \{\mathbf{e}^1, \mathbf{e}^2, \ldots, \mathbf{e}^n\}$ consisting of n basis vectors $\mathbf{e}^i$ by the requirement that the scalar product obeys

$$\delta^{j}_{i} = \mathbf{e}^i \cdot \mathbf{e}_j \equiv (\mathbf{e}^i, \mathbf{e}_j) \equiv \langle \mathbf{e}^i \mid \mathbf{e}_j \rangle = \begin{cases} 1 \text{ if } i = j \\ 0 \text{ if } i \neq j \end{cases}. \tag{5.18}$$

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 $\mathbf{e}^i \cdot \mathbf{e}_j \equiv (\mathbf{e}^i, \mathbf{e}_j) \equiv \langle \mathbf{e}^i \mid \mathbf{e}_j \rangle$ recall different notations of the scalar product.

Again, note that (see also below) the dual basis vectors of an orthonormal basis can be coded identically (i.e. one-to-one) as compared to the components of the original basis vectors; that is, in this case, the components of the dual basis vectors are just rearranged in the transposed form of the original basis vectors.

The entire tensor formalism developed so far can be applied to define *contravariant* tensors as multinear forms

$$\beta : \mathbb{R}^k \mapsto \mathbb{R} \tag{5.19}$$

by

$$\beta(\mathbf{x}^1, \mathbf{x}^2, \dots, \mathbf{x}^k) = \sum_{i_1=1}^{n} \sum_{i_2=1}^{n} \cdots \sum_{i_k=1}^{n} \Xi^1_{i_1} \Xi^2_{i_2} \dots \Xi^k_{i_k} \beta(\mathbf{e}^{i_1}, \mathbf{e}^{i_2}, \dots, \mathbf{e}^{i_k}). \tag{5.20}$$

The

$$B^{i_1 i_2 \cdots i_k} = \beta(\mathbf{e}^{i_1}, \mathbf{e}^{i_2}, \dots, \mathbf{e}^{i_k}) \tag{5.21}$$

are the *components* of the contravariant tensor β 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

$$g(f_i^*, f_j) = g(f^i, f_j) = \delta^i{}_j, \tag{5.22}$$

where again $\delta^i{}_j$ is Kronecker delta function, which is defined

$$\delta^i_j = \begin{cases} 0, & \text{for } i \neq j; \\ 1, & \text{for } i = j \end{cases}, \tag{5.23}$$

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*

$$\mathbf{e}'^j = \sum_i b^j_i \mathbf{e}^i, \tag{5.24}$$

where $\{b^j_i\} = b$ 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 (5.18) one can find the connection between the transformation of covariant and contravariant basis elements and thus tensor components; that is,

$$\delta^j_i = \mathbf{e}'_i \cdot \mathbf{e}'^j = (a^k_i \mathbf{e}_k) \cdot (b^j_l \mathbf{e}^l) = a^k_i b^j_l \mathbf{e}_k \cdot \mathbf{e}^l = a^k_i b^j_l \delta^l_k = a^k_i b^j_k, \tag{5.25}$$

and

$$b = a^{-1} = a'. \tag{5.26}$$

The entire argument concerning transformations of covariant tensors and components can be carried through to the contravariant case. Hence, the contravariant components transform as

$$\beta(\mathbf{e}'^{j_1},\mathbf{e}'^{j_2},\ldots,\mathbf{e}'^{j_k}) = \beta\left(\sum_{i_1=1}^{n} a'^{j_1}_{i_1}\mathbf{e}^{i_1}, \sum_{i_2=1}^{n} a'^{j_2}_{i_2}\mathbf{e}^{i_2},\ldots, \sum_{i_k=1}^{n} a'^{j_k}_{i_k}\mathbf{e}^{i_k}\right)$$
$$= \sum_{i_1=1}^{n}\sum_{i_2=1}^{n}\cdots\sum_{i_k=1}^{n} a'^{j_1}_{i_1} a'^{j_2}_{i_2}\cdots a'^{j_k}_{i_k}\beta(\mathbf{e}^{i_1},\mathbf{e}^{i_2},\ldots,\mathbf{e}^{i_k}) \tag{5.27}$$

or

$$B'^{j_1 j_2\cdots j_k} = \sum_{i_1=1}^{n}\sum_{i_2=1}^{n}\cdots\sum_{i_k=1}^{n} a'^{j_1}_{i_1} a'^{j_2}_{i_2}\cdots a'^{j_k}_{i_k} B^{i_1 i_2 \ldots i_k}. \tag{5.28}$$

5.5 Orthonormal bases

For orthonormal bases,

$$\delta^j_i = \mathbf{e}_i\cdot\mathbf{e}^j \Longleftrightarrow \mathbf{e}_i = \mathbf{e}^i, \tag{5.29}$$

and thus the two bases are identical

$$\mathfrak{B} = \mathfrak{B}^* \tag{5.30}$$

and formally any distinction between covariant and contravariant vectors becomes irrelevant. Conceptually, such a distinction persists, though.

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 refered to as “vector space with metric” or “geometry”) is a vector space with 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* is a functional $\mathbb{R}^n \mapsto \mathbb{R}$ with the following properties

- $||\mathbf{x}-\mathbf{y}|| = 0 \iff \mathbf{x}=\mathbf{y}$,
- $||\mathbf{x}-\mathbf{y}|| = ||\mathbf{y}-\mathbf{x}||$ (symmetry),
- $||\mathbf{x}-\mathbf{z}|| \le ||\mathbf{x}-\mathbf{y}|| + ||\mathbf{y}-\mathbf{z}||$ (triangle inequality).

5.7.2 Construction of a metric from a scalar product by metric tensor

The *metric* tensor is defined by the scalar product

$$g_{ij} = \mathbf{e}_i\cdot\mathbf{e}_j \equiv (\mathbf{e}_i,\mathbf{e}_j) \equiv \langle \mathbf{e}_i \mid \mathbf{e}_j\rangle. \tag{5.31}$$

and

$$g^{ij} = \mathbf{e}^i \cdot \mathbf{e}^j \equiv (\mathbf{e}^i, \mathbf{e}^j) \equiv \langle \mathbf{e}^i \mid \mathbf{e}^j \rangle. \tag{5.32}$$

By definition of the (dual) basis in Eq. (4.32) on page 45,

$$g^i{}_j = g^{il} g_{lj} = \delta^i{}_j. \tag{5.33}$$

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 easy to change a covarant tensor into a contravariant 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 basis vectors:

$$\mathbf{e}^i = A^{ij} \mathbf{e}_j. \tag{5.34}$$

Then,

$$g^{ik} = \mathbf{e}^i \cdot \mathbf{e}^k = (A^{ij} \mathbf{e}_j) \cdot \mathbf{e}^k = A^{ij} (\mathbf{e}_j \cdot \mathbf{e}^k) = A^{ij} \delta_j^k = A^{ik} \tag{5.35}$$

and thus

$$\mathbf{e}^i = g^{ij} \mathbf{e}_j \tag{5.36}$$

and

$$\mathbf{e}_i = g_{ij} \mathbf{e}^j. \tag{5.37}$$

Question: Show that, for orthonormal bases, the metric tensor can be represented as a Kronecker delta function in all basis (form invariant); i.e., $\delta_{ij}, \delta^i_j, \delta^j_i, \delta^{ij}$.

Question: Why is g a tensor? Show its multilinearity.

5.7.3 *What can the metric tensor do for us?*

Most often it is used to raise/lower the indices; i.e., to change from contravariant to covariant and conversely from covariant to contravariant.

In the previous section, the metric tensor has been derived from the scalar product. The converse is true as well. 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),

$$\mathbf{x} \cdot \mathbf{y} \equiv (\mathbf{x}, \mathbf{y}) \equiv \langle \mathbf{x} \mid \mathbf{y} \rangle = X^i \mathbf{e}_i \cdot Y^j \mathbf{e}_j = X^i Y^j \mathbf{e}_i \cdot \mathbf{e}_j = X^i Y^j g_{ij} = X^T g Y. \tag{5.38}$$

It also characterizes the length of a vector: in the above equation, set $\mathbf{y} = \mathbf{x}$. Then,

$$\mathbf{x} \cdot \mathbf{x} \equiv (\mathbf{x}, \mathbf{x}) \equiv \langle \mathbf{x} \mid \mathbf{x} \rangle = X^i X^j g_{ij} \equiv X^T g X, \tag{5.39}$$

and thus

$$||x|| = \sqrt{X^i X^j g_{ij}} = \sqrt{X^T g X}. \tag{5.40}$$

The square of an infinitesimal vector $ds = \{d\mathbf{x}^i\}$ is

$$(ds)^2 = g_{ij} d\mathbf{x}^i d\mathbf{x}^j = d\mathbf{x}^T g dx. \tag{5.41}$$

Question: Prove that $||\mathbf{x}||$ mediated by g is indeed a metric; that is, that g represents a *bilinear functional* $g(\mathbf{x},\mathbf{y}) = \mathbf{x}^i\mathbf{y}^j g_{ij}$ that is *symmetric*; that is, $g(\mathbf{x},\mathbf{y}) = g(\mathbf{x},\mathbf{y})$ and *nondegenerate*; 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 $g(\mathbf{x},\mathbf{y}) \neq 0$.

5.7.4 *Transformation of the metric tensor*

Insertion into the definitions and coordinate transformations (5.10) and (5.15) yields

$$g_{ij} = \mathbf{e}_i \cdot \mathbf{e}_j = a'^l_i \mathbf{e}'_l \cdot a'^m_j \mathbf{e}'_m = a'^l_i a'^m_j \mathbf{e}'_l \cdot \mathbf{e}'_m = a'^l_i a'^m_j g'_{lm} = \frac{\partial X'^l}{\partial X^i}\frac{\partial X'^m}{\partial X^j} g'_{lm}. \tag{5.42}$$

Conversely,

$$g'_{ij} = \mathbf{e}'_i \cdot \mathbf{e}'_j = a^l_i \mathbf{e}_l \cdot a^m_j \mathbf{e}_m = a^l_i a^m_j \mathbf{e}_l \cdot \mathbf{e}_m = a^l_i a^m_j g_{lm} = \frac{\partial X^l}{\partial X'^i}\frac{\partial X^m}{\partial X'^j} g_{lm}. \tag{5.43}$$

If the geometry (i.e., the basis) is locally orthonormal, $g_{lm} = \delta_{lm}$, then $g'_{ij} = \frac{\partial X^l}{\partial X'^i}\frac{\partial X_l}{\partial X'^j}$.

In terms of the *Jacobian matrix*

$$J \equiv J_{ij} = \frac{\partial X'^i}{\partial X^j} \equiv \begin{pmatrix} \frac{\partial X'^1}{\partial X^1} & \cdots & \frac{\partial X'^1}{\partial X^n} \\ \vdots & \ddots & \vdots \\ \frac{\partial X'^n}{\partial X^1} & \cdots & \frac{\partial X'^n}{\partial X^n} \end{pmatrix}, \tag{5.44}$$

the metric tensor in Eq. (5.42) can be rewritten as

$$g = J^T g' J \equiv g_{ij} = J_{li} J_{mj} g'_{lm}. \tag{5.45}$$

If the manifold is embedded into an Euclidean space, then $g'_{lm} = \delta_{lm}$ and $g = J^T J$.

The metric tensor and the Jacobian (determinant) are thus related by

$$\det g = (\det J^T)(\det g')(\det J). \tag{5.46}$$

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*[2].

[2] Ernst Snapper and Robert J. Troyer. *Metric Affine Geometry*. Academic Press, New York, 1971

n-dimensional Euclidean space

$$g \equiv \{g_{ij}\} = \text{diag}(\underbrace{1,1,\ldots,1}_{n \text{ times}}) \tag{5.47}$$

One application in physics is quantum mechanics, where n stands for the dimension of a complex Hilbert space. Some definitions can be 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

$$g \equiv \{g_{ij}\} = \text{diag}(1, -1) \tag{5.48}$$

Minkowski space of dimension n

In this case the metric tensor is called the Minkowski metric and is often denoted by "η":

$$\eta \equiv \{\eta_{ij}\} = \text{diag}(\underbrace{1, 1, \ldots, 1}_{n-1 \text{ times}}, -1) \tag{5.49}$$

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 [3].

[3] 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, 1967a; A. D. Alexandrov. Mappings of spaces with families of cones and space-time transformations. *Annali di Matematica Pura ed Applicata*, 103: 229–257, 1967b; 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*, 28:259–266, 1972; Walter Benz. *Geometrische Transformationen*. BI Wissenschaftsverlag, Mannheim, 1992; June A. Lester. Distance preserving transformations. In Francis Buekenhout, editor, *Handbook of Incidence Geometry*. 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

Negative Euclidean space of dimension n

$$g \equiv \{g_{ij}\} = \text{diag}(\underbrace{-1, -1, \ldots, -1}_{n \text{ times}}) \tag{5.50}$$

Artinian four-space

$$g \equiv \{g_{ij}\} = \text{diag}(+1, +1, -1, -1) \tag{5.51}$$

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 "η") $\text{diag}(1, 1, 1, -1)$ corresponding to "flat" space-time.

The best known non-flat metric is the Schwarzschild metric

$$g \equiv \begin{pmatrix} (1 - 2m/r)^{-1} & 0 & 0 & 0 \\ 0 & r^2 & 0 & 0 \\ 0 & 0 & r^2 \sin^2\theta & 0 \\ 0 & 0 & 0 & -(1 - 2m/r) \end{pmatrix} \tag{5.52}$$

with respect to the spherical space-time coordinates r, θ, ϕ, t.

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 79) $X'_1 = r$, $X'_2 = \theta$, $X'_3 = \varphi$. In terms of r, θ, φ, the cartesian coordinates can be written as $X_1 = r \sin\theta \cos\varphi \equiv X'_1 \sin X'_2 \cos X'_3$, $X_2 = r \sin\theta \sin\varphi \equiv X'_1 \sin X'_2 \sin X'_3$, $X_3 = r\cos\theta \equiv X'_1 \cos X'_2$. Furthermore, since we are dealing with the cartesian orthonormal basis, $g_{ij} = \delta_{ij}$; hence finally

$$g'_{ij} = \frac{\partial X^l}{\partial X'^i} \frac{\partial X_l}{\partial X'^j} \equiv \text{diag}(1, r^2, r^2 \sin^2\theta), \tag{5.53}$$

and

$$(ds)^2 = (dr)^2 + r^2(d\theta)^2 + r^2 \sin^2\theta (d\varphi)^2. \tag{5.54}$$

The expression $(ds)^2 = (dr)^2 + r^2(d\varphi)^2$ for polar coordinates in two dimensions (i.e., $n = 2$) is obtained by setting $\theta = \pi/2$ and $d\theta = 0$.

Computation of the metric tensor of the Moebius strip

Parameter representation of the Moebius strip:

$$\Phi(u, v) = \begin{pmatrix} (1 + v\cos\frac{u}{2})\sin u \\ (1 + v\cos\frac{u}{2})\cos u \\ v \sin\frac{u}{2} \end{pmatrix} \tag{5.55}$$

with $u \in [0, 2\pi]$ represents the position of the point on the circle, and $v \in [-a, a]$ $a > 0$, where $2a$ is the "width" of the Moebius strip.

$$\Phi_v = \frac{\partial\Phi}{\partial v} = \begin{pmatrix} \cos\frac{u}{2}\sin u \\ \cos\frac{u}{2}\cos u \\ \sin\frac{u}{2} \end{pmatrix} \tag{5.56}$$

$$\Phi_u = \frac{\partial\Phi}{\partial u} = \begin{pmatrix} -\frac{1}{2} v \sin\frac{u}{2}\sin u + \left(1 + v\cos\frac{u}{2}\right)\cos u \\ -\frac{1}{2} v \sin\frac{u}{2}\cos u - \left(1 + v\cos\frac{u}{2}\right)\sin u \\ \frac{1}{2} v \cos\frac{u}{2} \end{pmatrix} \tag{5.57}$$

$$\begin{aligned} (\frac{\partial\Phi}{\partial v})^T \frac{\partial\Phi}{\partial u} &= \begin{pmatrix} \cos\frac{u}{2}\sin u \\ \cos\frac{u}{2}\cos u \\ \sin\frac{u}{2} \end{pmatrix}^T \begin{pmatrix} -\frac{1}{2} v \sin\frac{u}{2}\sin u + \left(1 + v\cos\frac{u}{2}\right)\cos u \\ -\frac{1}{2} v \sin\frac{u}{2}\cos u - \left(1 + v\cos\frac{u}{2}\right)\sin u \\ \frac{1}{2} v \cos\frac{u}{2} \end{pmatrix} \\ &= -\frac{1}{2}\left(\cos\frac{u}{2}\sin^2 u\right) v \sin\frac{u}{2} - \frac{1}{2}\left(\cos\frac{u}{2}\cos^2 u\right) v \sin\frac{u}{2} \\ &\quad + \frac{1}{2}\sin\frac{u}{2} v \cos\frac{u}{2} = 0 \end{aligned} \tag{5.58}$$

$$(\frac{\partial\Phi}{\partial v})^T \frac{\partial\Phi}{\partial v} = \begin{pmatrix} \cos\frac{u}{2}\sin u \\ \cos\frac{u}{2}\cos u \\ \sin\frac{u}{2} \end{pmatrix}^T \begin{pmatrix} \cos\frac{u}{2}\sin u \\ \cos\frac{u}{2}\cos u \\ \sin\frac{u}{2} \end{pmatrix}$$

$$= \quad \cos^2\frac{u}{2}\sin^2 u + \cos^2\frac{u}{2}\cos^2 u + \sin^2\frac{u}{2} = 1 \qquad (5.59)$$

$$\begin{aligned}
\left(\frac{\partial\Phi}{\partial u}\right)^T\frac{\partial\Phi}{\partial u} &= \begin{pmatrix} -\frac{1}{2}v\sin\frac{u}{2}\sin u + \left(1+v\cos\frac{u}{2}\right)\cos u \\ -\frac{1}{2}v\sin\frac{u}{2}\cos u - \left(1+v\cos\frac{u}{2}\right)\sin u \\ \frac{1}{2}v\cos\frac{u}{2}\end{pmatrix}^T \begin{pmatrix} -\frac{1}{2}v\sin\frac{u}{2}\sin u + \left(1+v\cos\frac{u}{2}\right)\cos u \\ -\frac{1}{2}v\sin\frac{u}{2}\cos u - \left(1+v\cos\frac{u}{2}\right)\sin u \\ \frac{1}{2}v\cos\frac{u}{2}\end{pmatrix} \\
&= \frac{1}{4}v^2\sin^2\frac{u}{2}\sin^2 u + \cos^2 u + 2v\cos^2 u\cos\frac{u}{2} + v^2\cos^2 u\cos^2\frac{u}{2} \\
&\quad + \frac{1}{4}v^2\sin^2\frac{u}{2}\cos^2 u + \sin^2 u + 2v\sin^2 u\cos\frac{u}{2} + v^2\sin^2 u\cos^2\frac{u}{2} \\
&\quad + \frac{1}{4}v^2\cos^2\frac{1}{2}u = \frac{1}{4}v^2 + v^2\cos^2\frac{u}{2} + 1 + 2v\cos\frac{1}{2}u \\
&= \left(1+v\cos\frac{u}{2}\right)^2 + \frac{1}{4}v^2
\end{aligned} \qquad (5.60)$$

Thus the metric tensor is given by

$$\begin{aligned}
g'_{ij} &= \frac{\partial X^s}{\partial X'^i}\frac{\partial X^t}{\partial X'^j}g_{st} = \frac{\partial X^s}{\partial X'^i}\frac{\partial X^t}{\partial X'^j}\delta_{st} \\
&\equiv \begin{pmatrix} \Phi_u\cdot\Phi_u & \Phi_v\cdot\Phi_u \\ \Phi_v\cdot\Phi_u & \Phi_v\cdot\Phi_v \end{pmatrix} = \operatorname{diag}\left(\left(1+v\cos\frac{u}{2}\right)^2 + \frac{1}{4}v^2, 1\right).
\end{aligned} \qquad (5.61)$$

5.7.6 Decomposition of tensors

Although a tensor of rank n transforms like the tensor product of n tensors of rank 1, not all rank-n tensors can be decomposed into a single tensor product of n tensors of rank 1.

Nevertheless, by a generalized Schmidt decomposition (cf. page 66), any rank-n tensor can be decomposed into the sum of n^k tensor products of n tensors of rank 1.

5.7.7 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 (but maybe with different f).

Although form invariance is a gratifying feature, a tensor (field) needs not be form invariant. Indeed, while

$$S(x) \equiv \begin{pmatrix} x_2^2 & -x_1x_2 \\ -x_1x_2 & x_1^2 \end{pmatrix} \qquad (5.62)$$

is a form invariant tensor field with respect to the basis $\{(0,1),(1,0)\}$ and orthogonal transformations (rotations around the origin)

$$\begin{pmatrix} \cos\varphi & \sin\varphi \\ -\sin\varphi & \cos\varphi \end{pmatrix}, \tag{5.63}$$

$$T(x) \equiv \begin{pmatrix} x_2^2 & x_1 x_2 \\ x_1 x_2 & x_1^2 \end{pmatrix} \tag{5.64}$$

is not (please verify). This, however, does not mean that T is not a valid, "respectable" tensor field; it is just not form invariant under rotations.

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; tht is, the numbers or scalar functions, would be different.

Ultimately, these tensor coordinates are numbers; that is, scalars, which are encodings of a multilinear function. As these tensor components are scalars, they can thus 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 $\partial_i = \partial/\partial \mathbf{x}^i$.)

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 arguement. 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:

$$\begin{aligned} A_{i_1 i_2 \ldots i_s i_t \ldots i_k} = A_{i_1 i_2 \ldots i_t i_s \ldots i_k} \quad \Longrightarrow \quad A'_{j_1 i_2 \ldots j_s j_t \ldots j_k} &= a^{i_1}_{j_1} a^{i_2}_{j_2} \cdots a^{i_s}_{j_s} a^{i_t}_{j_t} \cdots a^{i_k}_{j_k} A_{i_1 i_2 \ldots i_s i_t \ldots i_k} \\ &= a^{i_1}_{j_1} a^{i_2}_{j_2} \cdots a^{i_s}_{j_s} a^{i_t}_{j_t} \cdots a^{i_k}_{j_k} A_{i_1 i_2 \ldots i_t i_s \ldots i_k} \\ &= a^{i_1}_{j_1} a^{i_2}_{j_2} \cdots a^{i_t}_{j_t} a^{i_s}_{j_s} \cdots a^{i_k}_{j_k} A_{i_1 i_2 \ldots i_t i_s \ldots i_k} \\ &= A'_{j_1 i_2 \ldots j_t j_s \ldots j_k} \end{aligned} \tag{5.65}$$

$$\begin{aligned} A_{i_1 i_2 \ldots i_s i_t \ldots i_k} = -A_{i_1 i_2 \ldots i_t i_s \ldots i_k} = \quad \Longrightarrow \quad A'_{j_1 i_2 \ldots j_s j_t \ldots j_k} &= a^{i_1}_{j_1} a^{i_2}_{j_2} \cdots a^{i_s}_{j_s} a^{i_t}_{j_t} \cdots a^{i_k}_{j_k} A_{i_1 i_2 \ldots i_s i_t \ldots i_k} \\ &= -a^{i_1}_{j_1} a^{i_2}_{j_2} \cdots a^{i_s}_{j_s} a^{i_t}_{j_t} \cdots a^{i_k}_{j_k} A_{i_1 i_2 \ldots i_t i_s \ldots i_k} \\ &= -a^{i_1}_{j_1} a^{i_2}_{j_2} \cdots a^{i_t}_{j_t} a^{i_s}_{j_s} \cdots a^{i_k}_{j_k} A_{i_1 i_2 \ldots i_t i_s \ldots i_k}. \\ &= -A'_{j_1 i_2 \ldots j_t j_s \ldots j_k} \end{aligned} \tag{5.66}$$

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 dont 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 invarince (at least in the 0'th order). Nevertheless, note 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. (4.124) on page 83) in the standard basis

$$
\begin{aligned}
|\Psi^-\rangle &= \frac{1}{\sqrt{2}}(|+-\rangle - |-+\rangle) \\
&\equiv \left(0, \frac{1}{\sqrt{2}}, -\frac{1}{\sqrt{2}}, 0\right) \\
&\equiv \frac{1}{2}\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & -1 & 0 \\ 0 & -1 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}.
\end{aligned}
\tag{5.67}
$$

$|\Psi^-\rangle$, 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 $\mathbb{C}^4$.

Why is $|\Psi^-\rangle$ not decomposable? In order to be able to answer this question, consider the most general two-partite state

$$
|\psi\rangle = \psi_{--}|--\rangle + \psi_{-+}|-+\rangle + \psi_{+-}|+-\rangle + \psi_{++}|++\rangle, \tag{5.68}
$$

with $\psi_{ij} \in \mathbb{C}$, and compare it to the most general state obtainable through products of single-partite states $|\phi_1\rangle = \alpha_-|-\rangle + \alpha_+|+\rangle$ $|\phi_2\rangle = \beta_-|-\rangle + \beta_+|+\rangle$ with $\alpha_i, \beta_i \in \mathbb{C}$; that is

$$
\begin{aligned}
|\phi\rangle &= |\phi_1\rangle|\phi_2\rangle \\
&= (\alpha_-|-\rangle + \alpha_+|+\rangle)(\beta_-|-\rangle + \beta_+|+\rangle) \\
&= \alpha_-\beta_-|--\rangle + \alpha_-\beta_+|-+\rangle + \alpha_+\beta_-|+-\rangle + \alpha_+\beta_+|++\rangle,
\end{aligned}
\tag{5.69}
$$

and compare $|\psi\rangle$ with $|\phi\rangle$. Since the two-partite basis states $|--\rangle \equiv (1,0,0,0)$, $|-+\rangle \equiv (0,1,0,0)$, $|+-\rangle \equiv (0,0,1,0)$, $|++\rangle \equiv (0,0,0,1)$ are linear independent (indeed, orthonormal), we obtain $\psi_{--} = \alpha_-\beta_-$, $\psi_{-+} = \alpha_-\beta_+$, $\psi_{+-} = \alpha_+\beta_-$, $\psi_{++} = \alpha_+\beta_+$ from that comparison. Hence, $\psi_{--}/\psi_{-+} = \beta_-/\beta_+ = \psi_{+-}/\psi_{++}$, and thus a necessary and sufficient condition for a two-partite state to be decomposable is that its amplitudes obey

$$
\psi_{--}\psi_{++} = \psi_{-+}\psi_{+-}. \tag{5.70}
$$

This is not satisfied for the Bell state $|\Psi^-\rangle$ in Eq. (5.67), because in this case $\psi_{--} = \psi_{++} = 0$ and $\psi_{-+} = -\psi_{+-} = 1/\sqrt{2}$. Such nondecomposability is in physics referred to as *entanglement* [4].

Note also that $|\Psi^-\rangle$ is a *singlet state*, as it is invariant under the rotations (if you do not believe this please check yourself)

$$\begin{aligned} |+\rangle &= e^{i\frac{\varphi}{2}}\left(\cos\frac{\theta}{2}|+'\rangle - \sin\frac{\theta}{2}|-'\rangle\right), \\ |-\rangle &= e^{-i\frac{\varphi}{2}}\left(\sin\frac{\theta}{2}|+'\rangle + \cos\frac{\theta}{2}|-'\rangle\right) \end{aligned} \tag{5.71}$$

in the spherical coordinates θ, φ defined earlier on page 79, 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 (5.17) and (5.21), 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 ta 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.

Consider the tensor field defined by its components

$$A_{ij}(x_1,x_2) = \begin{pmatrix} -x_1x_2 & -x_2^2 \\ x_1^2 & x_1x_2 \end{pmatrix}$$

with respect to the standard basis $\{(1,0),(0,1)\}$. Is A form invariant with respect to rotations around the origin? That is, A should be form invariant with repect to transformations $x_i' = a_{ij}x_j$ with

$$a_{ij} = \begin{pmatrix} \cos\varphi & \sin\varphi \\ -\sin\varphi & \cos\varphi \end{pmatrix}.$$

"Outer" transformation: The right hand term in $A'_{ij} = a_{ik}a_{jl}A_{kl}(x_n)$ can be rewritten as a product of three matrices; that is,

$$a_{ik}a_{jl}A_{kl}(x_n) = a_{ik}A_{kl}a_{jl} = a_{ik}A_{kl}\left(a^T\right)_{lj} \equiv a\cdot A\cdot a^T.$$

a^T stands for the transposed matrix; that is, $(a^T)_{ij} = a_{ji}$.

$$\begin{pmatrix} \cos\varphi & \sin\varphi \\ -\sin\varphi & \cos\varphi \end{pmatrix}\begin{pmatrix} -x_1x_2 & -x_2^2 \\ x_1^2 & x_1x_2 \end{pmatrix}\begin{pmatrix} \cos\varphi & -\sin\varphi \\ \sin\varphi & \cos\varphi \end{pmatrix} =$$

$$= \begin{pmatrix} -x_1x_2\cos\varphi + x_1^2\sin\varphi & -x_2^2\cos\varphi + x_1x_2\sin\varphi \\ x_1x_2\sin\varphi + x_1^2\cos\varphi & x_2^2\sin\varphi + x_1x_2\cos\varphi \end{pmatrix}\begin{pmatrix} \cos\varphi & -\sin\varphi \\ \sin\varphi & \cos\varphi \end{pmatrix} =$$

[4] 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`

$$
= \begin{pmatrix}
\begin{array}{c}\cos\varphi\left(-x_1x_2\cos\varphi + x_1^2\sin\varphi\right)+\\ +\sin\varphi\left(-x_2^2\cos\varphi + x_1x_2\sin\varphi\right)\end{array} & \begin{array}{c}-\sin\varphi\left(-x_1x_2\cos\varphi + x_1^2\sin\varphi\right)+\\ +\cos\varphi\left(-x_2^2\cos\varphi + x_1x_2\sin\varphi\right)\end{array}\\
\\
\begin{array}{c}\cos\varphi\left(x_1x_2\sin\varphi + x_1^2\cos\varphi\right)+\\ +\sin\varphi\left(x_2^2\sin\varphi + x_1x_2\cos\varphi\right)\end{array} & \begin{array}{c}-\sin\varphi\left(x_1x_2\sin\varphi + x_1^2\cos\varphi\right)+\\ +\cos\varphi\left(x_2^2\sin\varphi + x_1x_2\cos\varphi\right)\end{array}
\end{pmatrix} =
$$

$$
= \begin{pmatrix}
\begin{array}{c}x_1x_2\left(\sin^2\varphi - \cos^2\varphi\right)+\\ +\left(x_1^2 - x_2^2\right)\sin\varphi\cos\varphi\end{array} & \begin{array}{c}2x_1x_2\sin\varphi\cos\varphi\\ -x_1^2\sin^2\varphi - x_2^2\cos^2\varphi\end{array}\\
\\
\begin{array}{c}2x_1x_2\sin\varphi\cos\varphi+\\ +x_1^2\cos^2\varphi + x_2^2\sin^2\varphi\end{array} & \begin{array}{c}-x_1x_2\left(\sin^2\varphi - \cos^2\varphi\right)-\\ -\left(x_1^2 - x_2^2\right)\sin\varphi\cos\varphi\end{array}
\end{pmatrix}
$$

Let us now perform the "inner" transform

$$
x_i' = a_{ij}x_j \Longrightarrow \begin{array}{rcl} x_1' &=& x_1\cos\varphi + x_2\sin\varphi\\ x_2' &=& -x_1\sin\varphi + x_2\cos\varphi. \end{array}
$$

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

$$
\begin{array}{rcl}
-x_1'x_2' &=& -\left(x_1\cos\varphi + x_2\sin\varphi\right)\left(-x_1\sin\varphi + x_2\cos\varphi\right) =\\
&=& -\left(-x_1^2\sin\varphi\cos\varphi + x_2^2\sin\varphi\cos\varphi - x_1x_2\sin^2\varphi + x_1x_2\cos^2\varphi\right) =\\
&=& x_1x_2\left(\sin^2\varphi - \cos^2\varphi\right) + \left(x_1^2 - x_2^2\right)\sin\varphi\cos\varphi\\
(x_1')^2 &=& \left(x_1\cos\varphi + x_2\sin\varphi\right)\left(x_1\cos\varphi + x_2\sin\varphi\right) =\\
&=& x_1^2\cos^2\varphi + x_2^2\sin^2\varphi + 2x_1x_2\sin\varphi\cos\varphi\\
(x_2')^2 &=& \left(-x_1\sin\varphi + x_2\cos\varphi\right)\left(-x_1\sin\varphi + x_2\cos\varphi\right) =\\
&=& x_1^2\sin^2\varphi + x_2^2\cos^2\varphi - 2x_1x_2\sin\varphi\cos\varphi
\end{array}
$$

and hence

$$
A'(x_1', x_2') = \begin{pmatrix} -x_1'x_2' & -(x_2')^2\\ (x_1')^2 & x_1'x_2' \end{pmatrix}
$$

is invariant with respect to basis rotations

$$
\{(\cos\varphi, -\sin\varphi), (\sin\varphi, \cos\varphi)\}
$$

.

Incidentally, $A(x)$ can be written as the product of two invariant tensors $b_i(x)$ and $c_j(x)$:

$$
A_{ij}(x) = b_i(x)c_j(x),
$$

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:

$$
b_1c_1 = -x_1x_2 = A_{11},
$$

$$
\begin{aligned}
b_1 c_2 &= -x_2^2 = A_{12},\\
b_2 c_1 &= x_1^2 = A_{21},\\
b_2 c_2 &= x_1 x_2 = A_{22}.
\end{aligned}
$$

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 A is nonunique, since

$$
A(x_1,x_2) = \begin{pmatrix} -x_1 x_2 & -x_2^2 \\ x_1^2 & x_1 x_2 \end{pmatrix} = \begin{pmatrix} -x_2^2 \\ x_1 x_2 \end{pmatrix} \otimes \left(\frac{x_1}{x_2}, 1 \right).
$$

5.8 *The Kronecker symbol δ*

For vector spaces of dimension n the totally symmetric Kronecker symbol δ, sometimes referred to as the delta symbol δ–tensor, can be defined by

$$
\delta_{i_1 i_2 \cdots i_k} = \begin{cases} +1 & \text{if } i_1 = i_2 = \cdots = i_k \\ 0 & \text{otherwise (that is, some indices are not identical).} \end{cases} \tag{5.72}
$$

5.9 *The Levi-Civita symbol ε*

For vector spaces of dimension n the totally antisymmetric Levi-Civita symbol ε, sometimes referred to as the Levi-Civita symbol ε–tensor, can be defined by the number of permutations of its indices; that is,

$$
\varepsilon_{i_1 i_2 \cdots i_k} = \begin{cases} +1 & \text{if } (i_1 i_2 \dots i_k) \text{ is an } \textit{even} \text{ permutation of } (1,2,\dots k) \\ -1 & \text{if } (i_1 i_2 \dots i_k) \text{ is an } \textit{odd} \text{ permutation of } (1,2,\dots k) \\ 0 & \text{otherwise (that is, some indices are identical).} \end{cases} \tag{5.73}
$$

Hence, 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 $\mathbf{a} \equiv a_i$ and $\mathbf{b} \equiv b_i$ can be written as $\mathbf{a} \times \mathbf{b} \equiv \varepsilon_{ijk} a_j b_k$.

5.10 The nabla, Laplace, and D'Alembert operators

The *nabla operator*

$$\nabla = \left(\frac{\partial}{\partial x_1}, \frac{\partial}{\partial x_2}, \ldots, \frac{\partial}{\partial x_n} \right). \tag{5.74}$$

is a vector differential operator in an n-dimensional vector space $\mathfrak{V}$. In index notation, $\nabla_i = \partial_x = \partial_{x_i}$.

In three dimensions and in the standard Cartesian basis,

$$\nabla = \left(\frac{\partial}{\partial x_1}, \frac{\partial}{\partial x_2}, \frac{\partial}{\partial x_3} \right) = \mathbf{e}_1 \frac{\partial}{\partial x_1} + \mathbf{e}_2 \frac{\partial}{\partial x_2} + \mathbf{e}_3 \frac{\partial}{\partial x_3}. \tag{5.75}$$

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), (ii) the *divergence* of a vector field $\mathbf{v}(x_1, x_2, x_3)$ (rendering a scalar field), and (iii) the *curl* (rotation) of a vector field $\mathbf{v}(x_1, x_2, x_3)$ (rendering a vector field) as follows:

$$\operatorname{grad} f = \nabla f = \left(\frac{\partial f}{\partial x_1}, \frac{\partial f}{\partial x_2}, \frac{\partial f}{\partial x_3} \right), \tag{5.76}$$

$$\operatorname{div} \mathbf{v} = \nabla \cdot \mathbf{v} = \frac{\partial v_1}{\partial x_1} + \frac{\partial v_2}{\partial x_2} + \frac{\partial v_3}{\partial x_3}, \tag{5.77}$$

$$\operatorname{rot} \mathbf{v} = \nabla \times \mathbf{v} = \left(\frac{\partial v_3}{\partial x_2} - \frac{\partial v_2}{\partial x_3}, \frac{\partial v_1}{\partial x_3} - \frac{\partial v_3}{\partial x_1}, \frac{\partial v_2}{\partial x_1} - \frac{\partial v_1}{\partial x_2} \right). \tag{5.78}$$

The *Laplace operator* is defined by

$$\Delta = \nabla^2 = \nabla \cdot \nabla = \frac{\partial^2}{\partial^2 x_1} + \frac{\partial^2}{\partial^2 x_2} + \frac{\partial^2}{\partial^2 x_3}. \tag{5.79}$$

In special relativity and electrodynamics and wave theory, as well as in by the Minkowski space of dimension four, the *D'Alembert operator* is defined by the Minkowski metric $\eta = \operatorname{diag}(1, 1, 1, -1)$

$$\Box = \partial_i \partial^i = \eta_{ij} \partial^i \partial^j = \nabla^2 - \frac{\partial^2}{\partial^2 t} = \nabla \cdot \nabla - \frac{\partial^2}{\partial^2 t} = \frac{\partial^2}{\partial^2 x_1} + \frac{\partial^2}{\partial^2 x_2} + \frac{\partial^2}{\partial^2 x_3} - \frac{\partial^2}{\partial^2 t}. \tag{5.80}$$

5.11 Some tricks

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) $\frac{\partial X^i}{\partial X^j} = \delta^i_j$.

(iv) With the euclidean metric, $\frac{\partial X^i}{\partial X^i} = n$.

(v) For threedimensional vector spaces ($n = 3$) and the euclidean metric, the *Grassmann identity* holds:

$$\varepsilon_{ijk}\varepsilon_{klm} = \delta_{il}\delta_{jm} - \delta_{im}\delta_{jl}. \tag{5.81}$$

(vi) For threedimensional vector spaces ($n = 3$) and the euclidean metric, $|a\times b| = \sqrt{\varepsilon_{ijk}\varepsilon_{ist}a_j a_s b_k b_t} = \sqrt{|a|^2|b|^2 - (a\cdot b)^2} = \sqrt{\det\begin{pmatrix} a\cdot a & a\cdot b \\ a\cdot b & b\cdot b\end{pmatrix}} = |a||b|\sin\theta_{ab}$.

(vii) 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 $g_{ij} = \frac{\partial \Phi^k}{\partial X'^i}\frac{\partial \Phi^m}{\partial X'^j}\delta_{km}$.

5.12 *Some common misconceptions*

5.12.1 *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 rank-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 $(1,2)$.

5.12.2 *A matrix is a tensor*

See the above section.

Example (wrong!): A matrix is a tensor of rank 2.

Correct: with respect to the basis $\{(0,1),(1,0)\}$, a matrix represents a rank-2 tensor. The matrix components are the tensor components.

Consider the following examples in three-dimensional vector space. Let $r^2 = \sum_{i=1}^3 x_i^2$.

1.
$$\partial_j r = \partial_j \sqrt{\sum_i x_i^2} = \frac{1}{2}\frac{1}{\sqrt{\sum_i x_i^2}}2x_j = \frac{x_j}{r} \tag{5.82}$$

By using the chain rule one obtains

$$\partial_j r^\alpha = \alpha r^{\alpha-1}\left(\partial_j r\right) = \alpha r^{\alpha-1}\left(\frac{x_j}{r}\right) = \alpha r^{\alpha-2}x_j \tag{5.83}$$

and thus $\nabla r^\alpha = \alpha r^{\alpha-2}\mathbf{x}$.

2.
$$\partial_j \log r = \frac{1}{r}\left(\partial_j r\right) \tag{5.84}$$

With $\partial_j r = \frac{x_j}{r}$ derived earlier in Eq. (5.83) 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.

$$\partial_j\left[\left(\sum_i (x_i-a_i)^2\right)^{-\frac{1}{2}}+\left(\sum_i (x_i+a_i)^2\right)^{-\frac{1}{2}}\right]=$$
$$=-\frac{1}{2}\left[\frac{1}{\left(\sum_i (x_i-a_i)^2\right)^{\frac{3}{2}}}2\left(x_j-a_j\right)+\frac{1}{\left(\sum_i (x_i+a_i)^2\right)^{\frac{3}{2}}}2\left(x_j+a_j\right)\right]= \tag{5.85}$$
$$-\left(\sum_i (x_i-a_i)^2\right)^{-\frac{3}{2}}\left(x_j-a_j\right)-\left(\sum_i (x_i+a_i)^2\right)^{-\frac{3}{2}}\left(x_j+a_j\right).$$

4.

$$\nabla\left(\frac{\mathbf{r}}{r^3}\right)\equiv$$
$$\partial_i\left(\frac{r_i}{r^3}\right)=\frac{1}{r^3}\underbrace{\partial_i r_i}_{=3}+r_i\left(-3\frac{1}{r^4}\right)\left(\frac{1}{2r}\right)2r_i=3\frac{1}{r^3}-3\frac{1}{r^3}=0. \tag{5.86}$$

5. With the earlier solution (5.86) one obtains, for $r\neq 0$,

$$\Delta\left(\frac{1}{r}\right)\equiv$$
$$\partial_i\partial_i\frac{1}{r}=\partial_i\left(-\frac{1}{r^2}\right)\left(\frac{1}{2r}\right)2r_i=-\partial_i\frac{r_i}{r^3}=0. \tag{5.87}$$

6. With the earlier solution (5.86) one obtains

$$\Delta\left(\frac{\mathbf{rp}}{r^3}\right)\equiv$$
$$\partial_i\partial_i\frac{r_jp_j}{r^3}=\partial_i\left[\frac{p_i}{r^3}+r_jp_j\left(-3\frac{1}{r^5}\right)r_i\right]=$$
$$=p_i\left(-3\frac{1}{r^5}\right)r_i+p_i\left(-3\frac{1}{r^5}\right)r_i+ \tag{5.88}$$
$$+r_jp_j\left[\left(15\frac{1}{r^6}\right)\left(\frac{1}{2r}\right)2r_i\right]r_i+r_jp_j\left(-3\frac{1}{r^5}\right)\underbrace{\partial_i r_i}_{=3}=$$
$$=r_ip_i\frac{1}{r^5}(-3-3+15-9)=0$$

7. With $r\neq 0$ and constant $\mathbf{p}$ one obtains

Note that, in three dimensions, the Grassmann identity (5.81) $\varepsilon_{ijk}\varepsilon_{klm}=\delta_{il}\delta_{jm}-\delta_{im}\delta_{jl}$ holds.

$$\begin{aligned}
\nabla\times(\mathbf{p}\times\frac{\mathbf{r}}{r^3}) &\equiv \varepsilon_{ijk}\partial_j\varepsilon_{klm}p_l\frac{r_m}{r^3}=p_l\varepsilon_{ijk}\varepsilon_{klm}\left[\partial_j\frac{r_m}{r^3}\right]=\\
&= p_l\varepsilon_{ijk}\varepsilon_{klm}\left[\frac{1}{r^3}\partial_j r_m+r_m\left(-3\frac{1}{r^4}\right)\left(\frac{1}{2r}\right)2r_j\right]=\\
&= p_l\varepsilon_{ijk}\varepsilon_{klm}\left[\frac{1}{r^3}\delta_{jm}-3\frac{r_jr_m}{r^5}\right]=\\
&= p_l(\delta_{il}\delta_{jm}-\delta_{im}\delta_{jl})\left[\frac{1}{r^3}\delta_{jm}-3\frac{r_jr_m}{r^5}\right]=\\
&= p_i\underbrace{\left(3\frac{1}{r^3}-3\frac{1}{r^3}\right)}_{=0}-p_j\left(\frac{1}{r^3}\underbrace{\partial_j r_i}_{=\delta_{ij}}-3\frac{r_jr_i}{r^5}\right)=\\
&\equiv -\frac{\mathbf{p}}{r^3}+3\frac{(\mathbf{rp})\,\mathbf{r}}{r^5}.
\end{aligned}$$

8.

$$\begin{aligned}
&\nabla\times(\nabla\Phi)\\
&\equiv\varepsilon_{ijk}\partial_j\partial_k\Phi\\
&=\varepsilon_{ikj}\partial_k\partial_j\Phi\\
&=\varepsilon_{ikj}\partial_j\partial_k\Phi\\
&=-\varepsilon_{ijk}\partial_j\partial_k\Phi=0.
\end{aligned} \tag{5.89}$$

This is due to the fact that $\partial_j\partial_k$ is symmetric, whereas ε_{ijk} ist 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

$$
\begin{aligned}
&(\mathbf{x}\times\mathbf{y})\times\mathbf{z}\\
&\equiv \varepsilon_{ijl}\varepsilon_{jkm}x_k y_m z_l\\
&= -\varepsilon_{ilj}\varepsilon_{jkm}x_k y_m z_l\\
&= -(\delta_{ik}\delta_{lm}-\delta_{im}\delta_{lk})x_k y_m z_l\\
&= -x_i\mathbf{y}\cdot\mathbf{z}+y_i\mathbf{x}\cdot\mathbf{z}.
\end{aligned}
\tag{5.90}
$$

versus

$$
\begin{aligned}
&\mathbf{x}\times(\mathbf{y}\times\mathbf{z})\\
&\equiv \varepsilon_{ilj}\varepsilon_{jkm}x_l y_k z_m\\
&= (\delta_{ik}\delta_{lm}-\delta_{im}\delta_{lk})x_l y_k z_m\\
&= y_i\mathbf{x}\cdot\mathbf{z}-z_i\mathbf{x}\cdot\mathbf{y}.
\end{aligned}
\tag{5.91}
$$

10. Let $\mathbf{w}=\frac{\mathbf{p}}{r}$ with $p_i=p_i\left(t-\frac{r}{c}\right)$, whereby t and c are constants. Then,

$$
\begin{aligned}
\text{div}\mathbf{w} &= \nabla\cdot\mathbf{w}\\
\equiv \partial_i w_i &= \partial_i\left[\frac{1}{r}p_i\left(t-\frac{r}{c}\right)\right]=\\
&= \left(-\frac{1}{r^2}\right)\left(\frac{1}{2r}\right)2r_ip_i+\frac{1}{r}p_i'\left(-\frac{1}{c}\right)\left(\frac{1}{2r}\right)2r_i=\\
&= -\frac{r_ip_i}{r^3}-\frac{1}{cr^2}p_i'r_i.
\end{aligned}
$$

Hence, $\text{div}\mathbf{w}=\nabla\cdot\mathbf{w}=-\left(\frac{\mathbf{rp}}{r^3}+\frac{\mathbf{rp}'}{cr^2}\right)$.

$$
\begin{aligned}
\text{rot}\mathbf{w} &= \nabla\times\mathbf{w}\\
\varepsilon_{ijk}\partial_j w_k &= \equiv\varepsilon_{ijk}\left[\left(-\frac{1}{r^2}\right)\left(\frac{1}{2r}\right)2r_jp_k+\frac{1}{r}p_k'\left(-\frac{1}{c}\right)\left(\frac{1}{2r}\right)2r_j\right]=\\
&= -\frac{1}{r^3}\varepsilon_{ijk}r_jp_k-\frac{1}{cr^2}\varepsilon_{ijk}r_jp_k'=\\
&\equiv -\frac{1}{r^3}\left(\mathbf{r}\times\mathbf{p}\right)-\frac{1}{cr^2}\left(\mathbf{r}\times\mathbf{p}'\right).
\end{aligned}
$$

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:

$$
\int_V \nabla\cdot\mathbf{w}\,dv=\int_F \mathbf{w}\cdot d\mathbf{f}.
\tag{5.92}
$$

Consider the vector field $\mathbf{w}=(4x,-2y^2,z^2)$ and the (cylindric) volume bounded by the planes $x^2+y^2=4$, $z=0$ und $z=3$.

Let us first look at the left hand side $\int_V \nabla\cdot\mathbf{w}\,dv$ of Eq. (5.92):

$$
\nabla\mathbf{w}=\text{div}\,\mathbf{w}=4-4y+2z
$$

$$
\begin{aligned}
\Longrightarrow \int_V \text{div}\,\mathbf{w}\,dv &= \int_{z=0}^{3} dz \int_{x=-2}^{2} dx \int_{y=-\sqrt{4-x^2}}^{\sqrt{4-x^2}} dy\,\left(4-4y+2z\right) = \\
&\qquad \text{cylindric coordinates: } \begin{bmatrix} x &=& r\cos\varphi \\ y &=& r\sin\varphi \\ z &=& z \end{bmatrix} \\
&= \int_{z=0}^{3} dz \int_{0}^{2} r\,dr \int_{0}^{2\pi} d\varphi \left(4-4r\sin\varphi+2z\right) = \\
&= \int_{z=0}^{3} dz \int_{0}^{2} r\,dr \left(4\varphi+4r\cos\varphi+2\varphi z\right)\Big|_{\varphi=0}^{2\pi} = \\
&= \int_{z=0}^{3} dz \int_{0}^{2} r\,dr\,(8\pi+4r+4\pi z-4r) = \\
&= \int_{z=0}^{3} dz \int_{0}^{2} r\,dr\,(8\pi+4\pi z) \\
&= 2\left(8\pi z+4\pi\frac{z^2}{2}\right)\Big|_{z=0}^{z=3} = 2(24+18)\pi = 84\pi
\end{aligned}
$$

Now consider the right hand side $\int_F \mathbf{w}\cdot d\mathbf{f}$ of Eq. (5.92). The surface consists of three parts: the upper plane F_1 of the cylinder is characterized by $z=0$; the lower plane F_2 of the cylinder is characterized by $z=3$; the side area F_3 of the cylinder is characterized by $x^2+y^2=4$. $d\mathbf{f}$ must be normal to these surfaces, pointing outwards; hence

$$
\begin{aligned}
F_1: \int_{\mathscr{F}_1} \mathbf{w}\cdot d\mathbf{f}_1 &= \int_{\mathscr{F}_1} \begin{pmatrix} 4x \\ -2y^2 \\ z^2=0 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ -1 \end{pmatrix} dx\,dy = 0 \\
F_2: \int_{\mathscr{F}_2} \mathbf{w}\cdot d\mathbf{f}_2 &= \int_{\mathscr{F}_2} \begin{pmatrix} 4x \\ -2y^2 \\ z^2=9 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} dx\,dy = \\
&= 9\int_{K_{r=2}} df = 9\cdot 4\pi = 36\pi \\
F_3: \int_{\mathscr{F}_3} \mathbf{w}\cdot d\mathbf{f}_3 &= \int_{\mathscr{F}_3} \begin{pmatrix} 4x \\ -2y^2 \\ z^2 \end{pmatrix} \left(\frac{\partial\mathbf{x}}{\partial\varphi}\times\frac{\partial\mathbf{x}}{\partial z}\right) d\varphi\,dz \quad (r=2=\text{const.})
\end{aligned}
$$

$$
\frac{\partial\mathbf{x}}{\partial\varphi} = \begin{pmatrix} -r\sin\varphi \\ r\cos\varphi \\ 0 \end{pmatrix} = \begin{pmatrix} -2\sin\varphi \\ 2\cos\varphi \\ 0 \end{pmatrix};\quad \frac{\partial\mathbf{x}}{\partial z} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}
$$

$$
\Longrightarrow \left(\frac{\partial\mathbf{x}}{\partial\varphi}\times\frac{\partial\mathbf{x}}{\partial z}\right) = \begin{pmatrix} 2\cos\varphi \\ 2\sin\varphi \\ 0 \end{pmatrix}
$$

$$
\begin{aligned}
\Longrightarrow F_3 &= \int_{\varphi=0}^{2\pi} d\varphi \int_{z=0}^{3} dz \begin{pmatrix} 4\cdot 2\cos\varphi \\ -2(2\sin\varphi)^2 \\ z^2 \end{pmatrix} \begin{pmatrix} 2\cos\varphi \\ 2\sin\varphi \\ 0 \end{pmatrix} = \\
&= \int_{\varphi=0}^{2\pi} d\varphi \int_{z=0}^{3} dz \left(16\cos^2\varphi - 16\sin^3\varphi\right) = \\
&= 3\cdot 16 \int_{\varphi=0}^{2\pi} d\varphi \left(\cos^2\varphi - \sin^3\varphi\right) = \\
&= \left[\begin{array}{lcl} \int \cos^2\varphi\, d\varphi &=& \frac{\varphi}{2} + \frac{1}{4}\sin 2\varphi \\ \int \sin^3\varphi\, d\varphi &=& -\cos\varphi + \frac{1}{3}\cos^3\varphi \end{array}\right] = \\
&= 3\cdot 16 \left\{ \frac{2\pi}{2} - \underbrace{\left[\left(1+\frac{1}{3}\right) - \left(1+\frac{1}{3}\right)\right]}_{=0} \right\} = 48\pi
\end{aligned}
$$

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

$$
\int_{\mathscr{F}} \operatorname{rot} \mathbf{b}\cdot d\mathbf{f} = \oint_{\mathscr{C}_{\mathscr{F}}} \mathbf{b}\cdot d\mathbf{s}. \tag{5.93}
$$

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 $\int_{\mathscr{F}} \operatorname{rot}\mathbf{b}\cdot d\mathbf{f}$ of Eq. (5.93):

$$
\mathbf{b} = \begin{pmatrix} yz \\ -xz \\ 0 \end{pmatrix} \Longrightarrow \operatorname{rot}\mathbf{b} = \nabla\times\mathbf{b} = \begin{pmatrix} x \\ y \\ -2z \end{pmatrix}
$$

Let us transform this into spherical coordinates:

$$
\mathbf{x} = \begin{pmatrix} r\sin\theta\cos\varphi \\ r\sin\theta\sin\varphi \\ r\cos\theta \end{pmatrix}
$$

$$
\Rightarrow \frac{\partial\mathbf{x}}{\partial\theta} = r \begin{pmatrix} \cos\theta\cos\varphi \\ \cos\theta\sin\varphi \\ -\sin\theta \end{pmatrix}; \quad \frac{\partial\mathbf{x}}{\partial\varphi} = r \begin{pmatrix} -\sin\theta\sin\varphi \\ \sin\theta\cos\varphi \\ 0 \end{pmatrix}
$$

$$
d\mathbf{f} = \left(\frac{\partial\mathbf{x}}{\partial\theta}\times\frac{\partial\mathbf{x}}{\partial\varphi}\right) d\theta\, d\varphi = r^2 \begin{pmatrix} \sin^2\theta\cos\varphi \\ \sin^2\theta\sin\varphi \\ \sin\theta\cos\theta \end{pmatrix} d\theta\, d\varphi
$$

$$\nabla \times \mathbf{b} = r \begin{pmatrix} \sin\theta\cos\varphi \\ \sin\theta\sin\varphi \\ -2\cos\theta \end{pmatrix}$$

$$\begin{aligned}
\int_{\mathscr{F}} \text{rot}\,\mathbf{b}\cdot d\mathbf{f} &= \int_{\theta=0}^{\pi/4} d\theta \int_{\varphi=0}^{2\pi} d\varphi\, a^3 \begin{pmatrix} \sin\theta\cos\varphi \\ \sin\theta\sin\varphi \\ -2\cos\theta \end{pmatrix} \begin{pmatrix} \sin^2\theta\cos\varphi \\ \sin^2\theta\sin\varphi \\ \sin\theta\cos\theta \end{pmatrix} = \\
&= a^3 \int_{\theta=0}^{\pi/4} d\theta \int_{\varphi=0}^{2\pi} d\varphi \left[\sin^3\theta \underbrace{\left(\cos^2\varphi + \sin^2\varphi\right)}_{=1} - 2\sin\theta\cos^2\theta\right] = \\
&= 2\pi a^3 \left[\int_{\theta=0}^{\pi/4} d\theta \left(1-\cos^2\theta\right)\sin\theta - 2\int_{\theta=0}^{\pi/4} d\theta\sin\theta\cos^2\theta\right] = \\
&= 2\pi a^3 \int_{\theta=0}^{\pi/4} d\theta\sin\theta\left(1-3\cos^2\theta\right) = \\
&\quad \left[\begin{array}{l} \text{transformation of variables:} \\ \cos\theta = u \Rightarrow du = -\sin\theta d\theta \Rightarrow d\theta = -\frac{du}{\sin\theta} \end{array}\right] \\
&= 2\pi a^3 \int_{\theta=0}^{\pi/4} (-du)\left(1-3u^2\right) = 2\pi a^3 \left(\frac{3u^3}{3} - u\right)\Bigg|_{\theta=0}^{\pi/4} = \\
&= 2\pi a^3 \left(\cos^3\theta - \cos\theta\right)\Bigg|_{\theta=0}^{\pi/4} = 2\pi a^3 \left(\frac{2\sqrt{2}}{8} - \frac{\sqrt{2}}{2}\right) = \\
&= \frac{2\pi a^3}{8}\left(-2\sqrt{2}\right) = -\frac{\pi a^3\sqrt{2}}{2}
\end{aligned}$$

Now consider the right hand side $\oint_{\mathscr{C}_{\mathscr{F}}} \mathbf{b}\cdot d\mathbf{s}$ of Eq. (5.93). The radius r' of the circle surface $\{(x,y,z) \mid x,y \in \mathbb{R}, z = a/\sqrt{2}\}$ bounded by the spere with radius a is determined by $a^2 = (r')^2 + \frac{a}{2}$; hence, $r' = a/\sqrt{2}$. The curve of integration $\mathscr{C}_{\mathscr{F}}$ 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,

$$\mathbf{x} = a\begin{pmatrix} \frac{1}{\sqrt{2}}\cos\varphi \\ \frac{1}{\sqrt{2}}\sin\varphi \\ \frac{1}{\sqrt{2}} \end{pmatrix} = \frac{a}{\sqrt{2}}\begin{pmatrix} \cos\varphi \\ \sin\varphi \\ 1 \end{pmatrix} \in \mathscr{C}_{\mathscr{F}}$$

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

$$\oint_{\mathcal{C}_F} \mathbf{b} \cdot d\mathbf{s} = \frac{a^2}{2} \frac{a}{\sqrt{2}} \int_{\varphi=0}^{2\pi} \underbrace{\left(-\sin^2\varphi - \cos^2\varphi\right)}_{=-1} d\varphi = -\frac{a^3}{2\sqrt{2}} 2\pi = -\frac{a^3\pi}{\sqrt{2}}.$$

Part III:
Functional analysis

6
Brief review of complex analysis

The curriculum at the *Vienna University of Technology* includes complex analysis and Fourier analysis in the first year, so when taking this course in the second year, students need just to memorize these subjects. In what follows, a very brief review of complex analysis will therefore be presented.

For more detailed introductions to complex analysis, take, for instance, the classical book by Ahlfors [1], among a zillion other very good ones [2]. We shall study complex analysis not only for its beauty, but also because it yields very important analytical methods and tools; mainly for the computation of definite integrals. These methods will then be required for the computation of distributions and Green's functions, which will be reviewed later.

[1] 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

[2] 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; and Dietmar A. Salamon. *Funktionentheorie*. Birkhäuser, Basel, 2012. DOI: 10.1007/978-3-0348-0169-0. URL http://dx.doi.org/10.1007/978-3-0348-0169-0. see also URL http://www.math.ethz.ch/ salamon/PREPRINTS/cxana.pdf

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 it 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 $i^2 = -1$ be the solution of the equation $x^2 + 1 = 0$. Any complex number z can be decomposed into real numbers x, y, r and φ such that

$$z = \Re z + i \Im z = x + i y = r e^{i\varphi}, \tag{6.1}$$

with $x = r\cos\varphi$ and $y = r\sin\varphi$; where Euler's formula

$$e^{i\varphi} = \cos\varphi + i\sin\varphi \tag{6.2}$$

has been used. Note that, in particular, *Euler's identity*

$$e^{i\pi} = -1, \text{ or } e^{i\pi} + 1 = 0, \tag{6.3}$$

holds. For many mathematicians this is the "most beautiful" theorem [3].

[3] 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/BF03023741and 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

Euler's formula can be used to derive *de Moivre's formula* for integer n (for non-integer n the formula is multi-valued for different arguments φ):

$$e^{in\varphi} = (\cos\varphi + i\sin\varphi)^n = \cos(n\varphi) + i\sin(n\varphi). \tag{6.4}$$

If $z = \Re z$ we call z a real number. If $z = i\Im z$ we call z a purely imaginary number.

6.1 *Differentiable, holomorphic (analytic) function*

Consider the function $f(z)$ on the domain $G \subset \text{Domain}(f)$.

f is called *differentiable* or at the point z_0 if the differential quotient

$$\left.\frac{df}{dz}\right|_{z_0} = f'(z)\big|_{z_0} = \left.\frac{\partial f}{\partial x}\right|_{z_0} = \left.\frac{1}{i}\frac{\partial f}{\partial y}\right|_{z_0} \tag{6.5}$$

exists.

If f is differentiable in the entire domain G it is called *holomorphic*, or, used synonymuously, *analytic*.

6.2 *Cauchy-Riemann equations*

The function $f(z) = u(z) + iv(z)$ (where u and v are real valued functions) is analytic or holomorph if and only if $(a_b = \partial a/\partial b)$

$$u_x = v_y, \qquad u_y = -v_x \quad . \tag{6.6}$$

For a proof, differentiate along the real, and then along the complex axis, taking

$$\begin{aligned} f'(z) &= \lim_{x\to 0}\frac{f(z+x)-f(z)}{x} = \frac{\partial f}{\partial x} = \frac{\partial u}{\partial x} + i\frac{\partial v}{\partial x}, \text{ and}\\ f'(z) &= \lim_{y\to 0}\frac{f(z+iy)-f(z)}{iy} = \frac{\partial f}{\partial iy} = -i\frac{\partial f}{\partial y} = -i\frac{\partial u}{\partial y} + \frac{\partial v}{\partial y}. \end{aligned} \tag{6.7}$$

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

$$\frac{\partial u}{\partial x} + i\frac{\partial v}{\partial x} = -i\frac{\partial u}{\partial y} + \frac{\partial v}{\partial y}. \tag{6.8}$$

By comparing the real and imaginary parts of this equation, one obtains the two real Cauchy-Riemann equations

$$\begin{aligned} \frac{\partial u}{\partial x} &= \frac{\partial v}{\partial y},\\ \frac{\partial v}{\partial x} &= -\frac{\partial u}{\partial y}. \end{aligned} \tag{6.9}$$

6.3 *Definition analytical function*

Since 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

$$\begin{aligned}&\frac{\partial}{\partial x}\left(\frac{\partial u}{\partial x}\right)=\frac{\partial}{\partial x}\left(\frac{\partial v}{\partial y}\right)=\\&\frac{\partial}{\partial y}\left(\frac{\partial v}{\partial x}\right)=-\frac{\partial}{\partial y}\left(\frac{\partial u}{\partial y}\right),\text{ and}\\&\frac{\partial}{\partial y}\left(\frac{\partial u}{\partial x}\right)=\frac{\partial}{\partial y}\left(\frac{\partial v}{\partial y}\right)=\\&-\frac{\partial}{\partial x}\left(\frac{\partial v}{\partial x}\right)=\frac{\partial}{\partial x}\left(\frac{\partial u}{\partial y}\right),\end{aligned} \tag{6.10}$$

and thus

$$\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)u=0,\text{ and }\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)v=0 \quad . \tag{6.11}$$

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 $u_y = -v_x$

$$\nabla u(x,y)\cdot\nabla v(x,y)=\begin{pmatrix}u_x\\u_y\end{pmatrix}\cdot\begin{pmatrix}v_x\\v_y\end{pmatrix}=u_xv_x+u_yv_y=u_xv_x+(-v_x)u_x=0 \tag{6.12}$$

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

$$\left.\frac{d}{dt}f(z(t))\right|_{t=0}=\left.\frac{d}{dz}f(z)\right|_{z_0}\left.\frac{d}{dt}z(t)\right|_{t=0}\qquad=\lambda_0e^{i\varphi_0}\left.\frac{d}{dt}z(t)\right|_{t=0}. \tag{6.13}$$

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) λ_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 $\lambda_0e^{i\varphi_0}$.

6.4 *Cauchy's integral theorem*

If f is analytic on G and on its borders ∂G, then any closed line integral of f vanishes

$$\oint_{\partial G}f(z)dz=0 \quad . \tag{6.14}$$

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

$$\int_C f(z)dz = \int_a^b f(z(t))\frac{dz(t)}{dt}dt. \tag{6.15}$$

Let $f(z) = 1/z$ and $C : z(\varphi) = Re^{i\varphi}$, with $R > 0$ and $-\pi < \varphi \le \pi$. Then

$$\begin{aligned} \oint_{|z|=R} f(z)dz &= \int_{-\pi}^{\pi} f(z(\varphi))\frac{dz(\varphi)}{d\varphi}d\varphi \\ &= \int_{-\pi}^{\pi} \frac{1}{Re^{i\varphi}} R\, i\, e^{i\varphi} d\varphi \\ &= \int_{-\pi}^{\pi} i\varphi \\ &= 2\pi i \end{aligned} \tag{6.16}$$

is independent of R.

6.5 *Cauchy's integral formula*

If f is analytic on G and on its borders ∂G, then

$$f(z_0) = \frac{1}{2\pi i}\oint_{\partial G}\frac{f(z)}{z-z_0}dz \quad . \tag{6.17}$$

No proof is given here.

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 ∂G, then $\Longrightarrow$

$$f^{(n)}(z_0) = \frac{n!}{2\pi i}\oint_{\partial G}\frac{f(z)}{(z-z_0)^{n+1}}dz \quad . \tag{6.18}$$

No proof is given here.

Cauchy's integral formula presents a powerful method to compute integrals. Consider the following examples.

(i) For a starter, 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" ϵ

$$\begin{aligned} &\oint_{|z|=3} \frac{3z+2}{z(z+1)^3} dz \\ &= \oint_{|z|=\epsilon} \frac{3z+2}{z(z+1)^3} dz + \oint_{|z+1|=\epsilon} \frac{3z+2}{z(z+1)^3} dz \\ &= \oint_{|z|=\epsilon} \frac{3z+2}{(z+1)^3} \frac{1}{z} dz + \oint_{|z+1|=\epsilon} \frac{3z+2}{z} \frac{1}{(z+1)^3} dz \\ &= \frac{2\pi i}{0!} [[\frac{d^0}{dz^0}]] \frac{3z+2}{(z+1)^3}\Big|_{z=0} + \frac{2\pi i}{2!} \frac{d^2}{dz^2} \frac{3z+2}{z}\Big|_{z=-1} \\ &= \frac{2\pi i}{0!} \frac{3z+2}{(z+1)^3}\Big|_{z=0} + \frac{2\pi i}{2!} \frac{d^2}{dz^2} \frac{3z+2}{z}\Big|_{z=-1} \\ &= 4\pi i - 4\pi i \\ &= 0. \end{aligned} \tag{6.19}$$

(ii) Consider

$$\begin{aligned} &\oint_{|z|=3} \frac{e^{2z}}{(z+1)^4} dz \\ &= \frac{2\pi i}{3!} \frac{3!}{2\pi i} \oint_{|z|=3} \frac{e^{2z}}{(z-(-1))^{3+1}} dz \\ &= \frac{2\pi i}{3!} \frac{d^3}{dz^3} \left|e^{2z}\right|_{z=-1} \\ &= \frac{2\pi i}{3!} 2^3 \left|e^{2z}\right|_{z=-1} \\ &= \frac{8\pi i e^{-2}}{3}. \end{aligned} \tag{6.20}$$

Suppose $g(z)$ is a function with a pole of order n at the point z_0; that is

$$g(z) = \frac{f(z)}{(z-z_0)^n} \tag{6.21}$$

where $f(z)$ is an analytic function. Then,

$$\oint_{\partial G} g(z) dz = \frac{2\pi i}{(n-1)!} f^{(n-1)}(z_0) \quad . \tag{6.22}$$

6.6 *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*

$$f(z) = \sum_{k=-\infty}^{\infty} (z-z_0)^k a_k \tag{6.23}$$

The coefficients a_k are (the closed contour C must be in the concentric region)

$$a_k = \frac{1}{2\pi i} \oint_C (\chi - z_0)^{-k-1} f(\chi) d\chi \quad . \tag{6.24}$$

The coefficient

$$a_{-1} = \frac{1}{2\pi i} \oint_C f(\chi) d\chi \tag{6.25}$$

is called the *residue*, denoted by "Res."

No proof is given here.

Note that if $g(z)$ 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 $k \le -(n+1)$ vanish in the Laurent series. This follows from Cauchy's integral formula

$$a_k = \frac{1}{2\pi i} \oint_c (\chi - z_0)^{-k-n-1} h(\chi) d\chi = 0 \tag{6.26}$$

für $-k-n-1 \ge 0$.

6.7 *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,

$$\oint_{\partial G} f(z)dz = 2\pi i \sum_{z_i} \text{Res} f(z_i) \quad . \tag{6.27}$$

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 polynomials is

$$\text{deg}P(x) \le \text{deg}Q(x) - 2.$$

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

$$\int_{\curvearrowleft} R(z)dz = 0$$

in the upper (lower) complex plane

$$I = \int_{-\infty}^{\infty} R(z)dz + \int_{\curvearrowleft} R(z)dz = \oint_{\rightarrow \& \curvearrowleft} R(z)dz.$$

The added integral vanishes because it can be approximated by

$$\left| \int_{\curvearrowleft} R(z)dz \right| \le \lim_{r\to\infty} \left(\frac{\text{const.}}{r^2} \pi r \right) = 0.$$

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 "$\rightarrow \& \curvearrowleft$. "

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

$$\begin{aligned}
I &= \int_{-\infty}^{\infty} \tfrac{dx}{x^2+1} \\
&= \int_{-\infty}^{\infty} \tfrac{dz}{z^2+1} \\
&= \int_{-\infty}^{\infty} \tfrac{dz}{z^2+1} \int_{\curvearrowleft} \tfrac{dz}{z^2+1} \\
&= \int_{-\infty}^{\infty} \tfrac{dz}{(z+i)(z-i)} + \int_{\curvearrowleft} \tfrac{dz}{(z+i)(z-i)} \\
&= \oint \tfrac{1}{(z-i)} f(z)dz \text{ with } f(z) = \tfrac{1}{(z+i)} \\
&= 2\pi i \operatorname{Res}\left(\tfrac{1}{(z+i)(z-i)}\right)\Big|_{z=+i} \\
&= 2\pi i f(+i) \\
&= 2\pi i \tfrac{1}{(2i)} \\
&= \pi.
\end{aligned} \tag{6.28}$$

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)

$$\begin{aligned}
I &= \int_{-\infty}^{\infty} \tfrac{dx}{x^2+1} \\
&= \int_{-\infty}^{\infty} \tfrac{dz}{z^2+1} \\
&= \int_{-\infty}^{\infty} \tfrac{dz}{z^2+1} \int_{\text{lower path}} \tfrac{dz}{z^2+1} \\
&= \int_{-\infty}^{\infty} \tfrac{dz}{(z+i)(z-i)} + \int_{\text{lower path}} \tfrac{dz}{(z+i)(z-i)} \\
&= \oint \tfrac{1}{(z+i)} f(z)dz \text{ with } f(z) = \tfrac{1}{(z-i)} \\
&= 2\pi i \operatorname{Res}\left(\tfrac{1}{(z+i)(z-i)}\right)\Big|_{z=-i} \\
&= -2\pi i f(-i) \\
&= 2\pi i \tfrac{1}{(2i)} \\
&= \pi.
\end{aligned} \tag{6.29}$$

(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 $z = x + iy$, $e^{ipz} = e^{ipx}e^{-py} \to 0$ for $z \to \infty$ in the *upper* half plane. Hence, we can close the contour in the upper half plane and obtain with the help of the residue theorem.

If $a > 0$ only the pole at $z = +ia$ is enclosed in the contour; thus we obtain

$$\begin{aligned}
F(p) &= 2\pi i \operatorname{Res} \tfrac{e^{ipz}}{(z+ia)}\Big|_{z=+ia} \\
&= 2\pi i \tfrac{e^{i^2 pa}}{2ia} \\
&= \tfrac{\pi}{a} e^{-pa}.
\end{aligned} \tag{6.30}$$

If $a < 0$ only the pole at $z = -ia$ is enclosed in the contour; thus we obtain

$$\begin{aligned} F(p) &= 2\pi i \text{Res} \frac{e^{ipz}}{(z-ia)}\Big|_{z=-ia} \\ &= 2\pi i \frac{e^{-i^2pa}}{-2ia} \\ &= \frac{\pi}{-a} e^{-i^2pa} \\ &= \frac{\pi}{-a} e^{pa}. \end{aligned} \tag{6.31}$$

Hence, for $a \neq 0$,

$$F(p) = \frac{\pi}{|a|} e^{-|pa|}. \tag{6.32}$$

For $p < 0$ a very similar consideration, taking the *lower* path for continuation – and thus aquiring a minus sign because of the "clockwork" orientation of the path as compared to its interior – yields

$$F(p) = \frac{\pi}{|a|} e^{-|pa|}. \tag{6.33}$$

(iii) Not all singularities are "nice" poles. Consider

$$\oint_{|z|=1} e^{\frac{1}{z}} dz.$$

That is, 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. and 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. In such a case the residue can be found only by using Laurent series of $f(z)$; that is by *comparing* its coefficient of the $1/z$ term. Hence, $\text{Res}\left(e^{\frac{1}{z}}\right)\Big|_{z=0}$ is the coefficient 1 of the $1/z$ term. The residue is *not*, with $z = e^{i\varphi}$,

$$\begin{aligned} a_{-1} = & \text{ Res}\left(e^{\frac{1}{z}}\right)\Big|_{z=0} \\ \neq & \frac{1}{2\pi i} \oint_C e^{\frac{1}{z}} dz \\ & = \frac{1}{2\pi i} \int_{-\pi}^{\pi} e^{\frac{1}{e^{i\varphi}}} \frac{dz(\varphi)}{d\varphi} d\varphi \\ & = \frac{1}{2\pi i} \int_{-\pi}^{\pi} e^{\frac{1}{e^{i\varphi}}} i e^{i\varphi} d\varphi \\ & = \frac{1}{2\pi} \int_{-\pi}^{\pi} e^{-e^{i\varphi}} e^{i\varphi} d\varphi \\ & = \frac{1}{2\pi} \int_{-\pi}^{\pi} e^{-e^{i\varphi}+i\varphi} d\varphi \\ & = \frac{1}{2\pi} \int_{-\pi}^{\pi} i \frac{d}{d\varphi} e^{-e^{i\varphi}} d\varphi \\ & = \frac{i}{2\pi} e^{-e^{i\varphi}}\Big|_{-\pi}^{\pi} \\ & = 0. \end{aligned} \tag{6.34}$$

Why?

Thus, by the residue theorem,

$$\oint_{|z|=1} e^{\frac{1}{z}}\,dz = 2\pi i \,\text{Res}\,\left(e^{\frac{1}{z}}\right)\Big|_{z=0} = 2\pi i. \tag{6.35}$$

For $f(z) = e^{-\frac{1}{z}}$, the same argument yields $\text{Res}\,\left(e^{-\frac{1}{z}}\right)\Big|_{z=0} = -1$ and thus $\oint_{|z|=1} e^{-\frac{1}{z}}\,dz = -2\pi i$.

6.8 *Multi-valued relationships, branch points and 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 multifunction 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.

6.9 *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.

7
Brief review of Fourier transforms

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 [1] attempts to decompose a function into its constituent frequencies, known as a frequency spectrum. More formally, the goal is the expansion of periodic and aperiodic functions into periodic ones.

[1] 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

A function f is *periodic* if there exist a period $L \in \mathbb{R}$ such that, for all x in the domain of f,

$$f(L + x) = f(x). \tag{7.1}$$

Suppose that a function is periodic in the interval $[-L, L]$ with period $2L$. 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*

$$\begin{aligned}
f(x) &= \frac{a_0}{2} + \sum_{n=1}^{\infty} \left[a_n \cos\left(\frac{n\pi x}{L}\right) + b_n \sin\left(\frac{n\pi x}{L}\right) \right] \\
a_n &= \frac{1}{L} \int_{-L}^{L} dx f(x) \cos(nx) \qquad n \geq 0 \\
b_n &= \frac{1}{L} \int_{-L}^{L} dx f(x) \sin(nx) \qquad n > 0
\end{aligned}$$

Suppose again that a function is periodic in the interval $[-\pi, \pi]$ with period 2π. 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

$$f(x) = \sum_{k=-\infty}^{\infty} c_k e^{ikx}, \text{ with } c_k = \frac{1}{2\pi} \int_{-\pi}^{\pi} f(x) e^{-ikx} dx. \tag{7.2}$$

More generally, let f be a periodic function in the interval $[-\mathfrak{L}2, \mathfrak{L}2]$ with period L (we later consider the limit $L \to \infty$). Then, with

$$x \to \frac{2\pi}{L} x,$$

under similar "mild" conditions as mentioned earlier f can be decomposed into a *Fourier series*

$$f(x)=\sum_{k=-\infty}^{\infty} c_k e^{\frac{2\pi i k x}{L}}, \text{ with } c_k=\frac{1}{L}\int_{-\frac{1}{L}}^{\frac{1}{L}} f(x)e^{-i\frac{2\pi i k x}{L}}dx. \tag{7.3}$$

With the definition $\check{k}=2\pi k/L$, Eqs. (7.6) can be combined into

$$f(x)=\frac{1}{L}\sum_{k=-\infty}^{\infty}\int_{-\frac{1}{L}}^{\frac{1}{L}} f(x')e^{-i\check{k}(x'-x)}dx'. \tag{7.4}$$

Let us compute the Fourier series of

$$f(x)=\begin{cases}-x, & \text{für } -\pi\le x<0;\\ +x, & \text{für } 0\le x\le \pi.\end{cases}$$

$$\begin{aligned}
f(x) &= \frac{a_0}{2}+\sum_{n=1}^{\infty}\left[a_n\cos(nx)+b_n\sin(nx)\right]\\
a_n &= \frac{1}{\pi}\int_{-\pi}^{\pi} dx f(x)\cos(nx) \qquad n\ge 0\\
b_n &= \frac{1}{\pi}\int_{-\pi}^{\pi} dx f(x)\sin(nx) \qquad n>0
\end{aligned}$$

$f(x)=f(-x)$; that is, f is an even function of x; hence $b_n=0$.

$\underline{n=0:}$ $a_0=\frac{1}{\pi}\int_{-\pi}^{\pi} dx f(x)=\frac{2}{\pi}\int_0^{\pi} x dx=\pi.$

$\underline{n>0:}$

$$\begin{aligned}
a_n &= \frac{1}{\pi}\int_{-\pi}^{\pi} f(x)\cos(nx)dx=\frac{2}{\pi}\int_0^{\pi} x\cos(nx)dx=\\
&= \frac{2}{\pi}\left[\frac{\sin(nx)}{n}x\Big|_0^{\pi}-\int_0^{\pi}\frac{\sin(nx)}{n}dx\right]=\frac{2}{\pi}\frac{\cos(nx)}{n^2}\Big|_0^{\pi}=\\
&= \frac{2}{\pi}\frac{\cos(n\pi)-1}{n^2}=-\frac{4}{\pi n^2}\sin^2\frac{n\pi}{2}=\begin{cases}0 & \text{for even } n\\ -\frac{4}{\pi n^2} & \text{for odd } n\end{cases}
\end{aligned}$$

$$\begin{aligned}
\Longrightarrow f(x) &= \frac{\pi}{2}-\frac{4}{\pi}\left(\cos x+\frac{\cos 3x}{9}+\frac{\cos 5x}{25}+\cdots\right)=\\
&= \frac{\pi}{2}-\frac{4}{\pi}\sum_{n=0}^{\infty}\frac{\cos[(2n+1)x]}{(2n+1)^2}
\end{aligned}$$

Furthermore, define $\Delta\check{k}=2\pi/L$. Then Eq. (7.4) can be written as

$$f(x)=\frac{1}{2\pi}\sum_{k=-\infty}^{\infty}\int_{-\frac{1}{L}}^{\frac{1}{L}} f(x')e^{-i\check{k}(x'-x)}dx'\Delta\check{k}. \tag{7.5}$$

Now, in the "aperiodic" limit $L \to \infty$ we obtain the *Fourier transformation*

$$\begin{aligned} f(x) &= \frac{1}{2\pi}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} f(x')e^{-i\check{k}(x'-x)}\,dx'\,d\check{k}, \text{ or} \\ f(x) &= \int_{-\infty}^{\infty}\tilde{f}(k)e^{ikx}\,dk, \text{ and} \\ \tilde{f}(k) &= \int_{-\infty}^{\infty} f(x)e^{-ikx}\,dx. \end{aligned} \tag{7.6}$$

Let us compute the Fourier transform of the Gaussian

$$f(x) = e^{-x^2} \quad .$$

Hint: e^{-t^2} is analytic in the region $-k \le \mathrm{Im}\, t \le 0$; also

$$\int_{-\infty}^{\infty} dt e^{-t^2} = \pi^{1/2} \quad .$$

$$\begin{aligned} \tilde{f}(k) &= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dx e^{-x^2} e^{ikx} = \text{(completing the exponent)} \\ &= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dx e^{-\frac{k^2}{4}} e^{-\left(x-\frac{i}{2}k\right)^2} \end{aligned}$$

Variable transformation: $t = x - \frac{i}{2}k \Longrightarrow dt = dx \Longrightarrow$

$$\tilde{f}(k) = \frac{e^{-\frac{k^2}{4}}}{\sqrt{2\pi}} \int_{-\infty - i\frac{k}{2}}^{+\infty - i\frac{k}{2}} dt e^{-t^2}$$

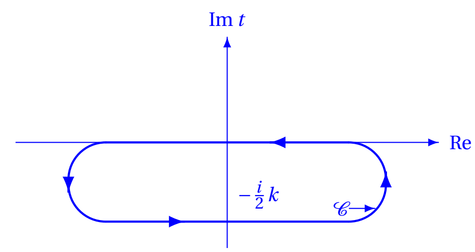


Figure 7.1: Integration path to compute the Fourier transform of the Gaussian.

$$\oint_{\mathscr{C}} dt e^{-t^2} = \int_{+\infty}^{-\infty} dt e^{-t^2} + \int_{-\infty-\frac{i}{2}k}^{+\infty-\frac{i}{2}k} dt e^{-t^2} = 0,$$

because e^{-t^2} is analytic in the region $-k \le \mathrm{Im}\, t \le 0$.

$$\Longrightarrow \int_{-\infty-\frac{i}{2}k}^{+\infty-\frac{i}{2}k} dt e^{-t^2} = \int_{-\infty}^{+\infty} dt e^{-t^2}$$

$$\tilde{f}(k) = \frac{1}{\sqrt{2\pi}} e^{-\frac{k^2}{4}} \underbrace{\int_{-\infty}^{+\infty} dt e^{-t^2}}_{\sqrt{\pi}} = \frac{e^{-\frac{k^2}{4}}}{\sqrt{2}}.$$

8
Distributions as generalized functions

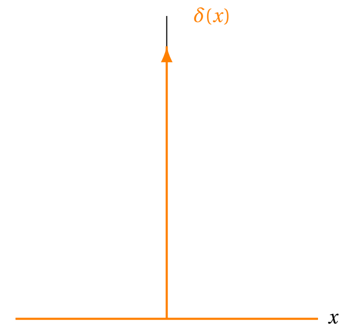


Figure 8.1: Dirac's δ-function as a "needle shaped" generalized function.

In the days when Dirac developed quantum mechanics, there was a need to define "singular scalar products" such as "$\langle x \mid y\rangle = \delta(x-y)$," with some generalization of the Kronecker delta function δ_{ij} which is zero whenever $x \neq y$ and "large enough" needle shaped (see Fig. 8.1) to yield unity when integrated over the entire reals; that is, "$\int_{-\infty}^{\infty}\langle x \mid y\rangle dy = \int_{-\infty}^{\infty}\delta(x-y)dy = 1$."

One of the first attempts to formalize these objects 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,

$$\delta_n(x-y) = \begin{cases} n & \text{for } y-\frac{1}{2n} < x < y+\frac{1}{2n} \\ 0 & \text{else} \end{cases} \tag{8.1}$$

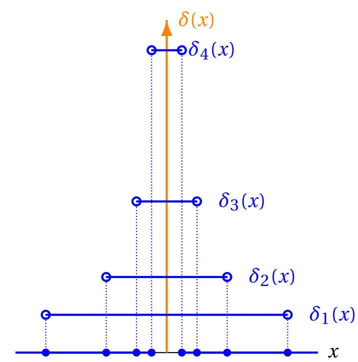


Figure 8.2: Delta sequence approximating Dirac's δ-function as a more and more "needle shaped" generalized function.

become the delta function $\delta(x-y)$. That is, in the fuctional sense (see below)

$$\lim_{n\to\infty}\delta_n(x-y) = \delta(x-y). \tag{8.2}$$

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.

Other delta sequences are

$$\begin{aligned}
\delta_n(x) &= \frac{n}{\sqrt{\pi}}e^{-n^2x^2}, && (8.3)\\
&= \frac{1}{\pi}\frac{\sin(nx)}{x}, && (8.4)\\
&= = (1\mp i)\left(\frac{n}{2\pi}\right)^{\frac{1}{2}} e^{\pm inx^2} && (8.5)\\
&= \frac{1}{\pi x}\frac{e^{inx}-e^{-inx}}{2i}, && (8.6)\\
&= \frac{1}{\pi}\frac{ne^{-x^2}}{1+n^2x^2}, && (8.7)\\
&= \frac{1}{2\pi}\int_{-n}^{n} e^{ixt}dt = \frac{1}{2\pi i x}\left. e^{ixt}\right|_{-n}^{n}, && (8.8)\\
&= \frac{1}{2\pi}\frac{\sin\left[\left(n+\frac{1}{2}\right)x\right]}{\sin\left(\frac{1}{2}x\right)}, && (8.9)
\end{aligned}$$

$$= \frac{1}{\pi}\frac{n}{1+n^2x^2}, \quad (8.10)$$
$$= \frac{n}{\pi}\left(\frac{\sin(nx)}{nx}\right)^2. \quad (8.11)$$

Other commonly used limit forms of the δ-function are the Gaussian, Lorentzian, and Dirichlet forms

$$\delta_\epsilon(x) = \lim_{\epsilon\to 0}\frac{1}{\sqrt{\pi}\epsilon}e^{-\frac{x^2}{\epsilon^2}}, \quad (8.12)$$
$$= \lim_{\epsilon\to 0}\frac{1}{\pi}\frac{\epsilon}{x^2+\epsilon^2}, \quad (8.13)$$
$$= \lim_{\epsilon\to 0}\frac{1}{\pi x}\sin\epsilon x, \quad (8.14)$$

respectively. Again, the limit

$$\delta(x) = \lim_{\epsilon\to 0}\delta_\epsilon(x) \quad (8.15)$$

has to be understood in the functional sense (see below).

Naturally, such "needle shaped functions" were viewed suspiciouly by many mathematicians at first, but later they embraced these types of functions [1] by developing a theory of *functional analysis* or *distributions*.

Distributions q are quasi-functions of one or more variables which can be interpreted in the "weak sense" as *functionals*; that is, by integrating them with suitable, "good" test functions φ of the class D of test functions

$$F(\varphi) = \int_{-\infty}^{\infty} q(x)\varphi(x)dx. \quad (8.16)$$

Recall that a functional is some mathematical entity which maps a function or another mathematical object into scalars in a linear manner; that is,

$$F(c_1\varphi_1 + c_2\varphi_2) = c_1F(\varphi_1) + c_2F(c_2\varphi_2\varphi_2). \quad (8.17)$$

In particular, the δ function maps to

$$F(\varphi) = \int_{-\infty}^{\infty}\delta(x-y)\varphi(x)dx = \varphi(y). \quad (8.18)$$

Let us see if 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. (8.1) and depicted in Fig. 8.2 is a delta sequence; that is, if, for large n, it converges to δ 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 $n\to\infty$; if the result is $\varphi(0)$, then we can identify $\delta_n(x)$ in this limit

[1] I. M. Gel'fand and G. E. Shilov. *Generalized Functions. Vol. 1: Properties and Operations*. Academic Press, New York, 1964. Translated from the Russian by Eugene Saletan

with $\delta(x)$ (in the functional sense).

$$\begin{aligned}
&\lim_{n\to\infty}\int_{-\infty}^{\infty}\delta_n(x)\varphi(x)dx \\
&\quad=\lim_{n\to\infty}\int_{-\frac{1}{2n}}^{\frac{1}{2n}} n\varphi(x)dx \\
&\qquad\text{[variable transformation:} \\
&\qquad\quad u=2n(x-y), x=\tfrac{u}{2n}+y, \\
&\qquad\quad du=2ndx, -1\le u\le 1] \\
&\quad=\lim_{n\to\infty}\int_{-1}^{1} n\varphi(\tfrac{u}{2n}+y)\tfrac{du}{2n} \\
&\quad=\lim_{n\to\infty}\tfrac{1}{2}\int_{-1}^{1}\varphi(\tfrac{u}{2n}+y)du \\
&\quad=\tfrac{1}{2}\int_{-1}^{1}\lim_{n\to\infty}\varphi(\tfrac{u}{2n}+y)du \\
&\quad=\tfrac{1}{2}\varphi(y)\int_{-1}^{1}du \\
&\quad=\varphi(y).
\end{aligned} \tag{8.19}$$

Hence, in the functional sense, this limit yields the δ-function.

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 impemented 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 $\int u'v = \int(uv)' - \int uv'$. By identifying u with the generalized function g (such as, for instance δ), and v with the test function φ, respectively, we obtain

$$\begin{aligned}
&\int_{-\infty}^{\infty} g'(x)\varphi(x)dx \\
&\quad= g(x)\varphi(x)\big|_{-\infty}^{\infty} - \int_{-\infty}^{\infty} g(x)\varphi'(x)dx \\
&\quad= g(\infty)\varphi(\infty) - g(-\infty)\varphi(-\infty) - \int_{-\infty}^{\infty} g(x)\varphi'(x)dx.
\end{aligned} \tag{8.20}$$

We can see here the two main requirements for “good” test functions:

1. that they vanish at infinity – that is, that their support (the set of arguments x where $g(x)\neq 0$) is finite; and

2. that they are continuosly differentiable – indeed, by induction, that they are arbitrarily often differentiable.

Hence we assume [2] that the tests functions φ are infinitely often differentiable, and 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,

$$\varphi_{\sigma,a}(x) = \begin{cases} e^{-\frac{1}{1-((x-a)/\sigma)^2}} & \text{for } |\frac{x-a}{\sigma}| < 1; \\ 0 & \text{else.} \end{cases} \tag{8.21}$$

In order to show that $\varphi_{\sigma,a}$ is a suitable test function, we have to proof its infinite differetiability, as well as the compactness of its support $M_{\varphi_{\sigma,a}}$. Let

$$\varphi_{\sigma,a}(x) := \varphi\left(\frac{x-a}{\sigma}\right)$$

[2] Laurent Schwartz. *Introduction to the Theory of Distributions*. University of Toronto Press, Toronto, 1952. collected and written by Israel Halperin

and thus

$$\varphi(x) = \begin{cases} e^{-\frac{1}{1-x^2}} & \text{for} \quad |x| < 1 \\ 0 & \text{for} \quad |x| \geq 1 \end{cases}$$

This function is drawn in Fig. 8.3.

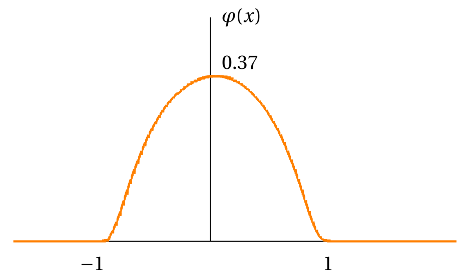


Figure 8.3: Plot of a test function $\varphi(x)$.

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

$$\varphi^{(n)}(x) = \begin{cases} \frac{P_n(x)}{(x^2-1)^{2n}} e^{\frac{1}{x^2-1}} & \text{for } |x| < 1 \\ 0 & \text{for } |x| \geq 1, \end{cases}$$

where $P_n(x)$ is a finite polynomial in x ($\varphi(u) = e^u \Longrightarrow \varphi'(u) = \frac{d\varphi}{du}\frac{du}{dx^2}\frac{dx^2}{dx} = \varphi(u)\left(-\frac{1}{(x^2-1)^2}\right)2x$ etc.) and $[x = 1-\varepsilon] \Longrightarrow x^2 = 1 - 2\varepsilon + \varepsilon^2 \Longrightarrow x^2 - 1 = \varepsilon(\varepsilon - 2)$

$$\begin{aligned} \lim_{x\uparrow 1} \varphi^{(n)}(x) &= \lim_{\varepsilon\downarrow 0} \frac{P_n(1-\varepsilon)}{\varepsilon^{2n}(\varepsilon-2)^{2n}} e^{\frac{1}{\varepsilon(\varepsilon-2)}} = \\ &= \lim_{\varepsilon\downarrow 0} \frac{P_n(1)}{\varepsilon^{2n}2^{2n}} e^{-\frac{1}{2\varepsilon}} = \left[\varepsilon = \frac{1}{R}\right] = \lim_{R\to\infty} \frac{P_n(1)}{2^{2n}} R^{2n} e^{-\frac{R}{2}} = 0, \end{aligned}$$

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 und g on B coincide in the points z_n, then they coincide on the entire domain B.

Not, 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, φ cannot be analytic. Indeed, $\varphi_{\sigma,\vec{a}}(x)$ diverges at $x = a \pm \sigma$. Hence $\varphi(x)$ cannot be Taylor expanded, and

$$C^\infty(\mathbb{R}^k) \underset{\Longleftarrow}{\overset{\not\Longrightarrow}{}} \text{analytic function} \quad (\text{"}C^\infty(\mathbb{C}^k)\text{"})$$

Other "good" test function are [3]

$$\left\{\phi_{c,d}(x)\right\}^{\frac{1}{n}} \tag{8.22}$$

obtained by choosing $n \in \mathbb{N} - 0$ and $a \leq c < d \leq b$ and by defining

$$\phi_{c,d}(x) = \begin{cases} e^{-\left(\frac{1}{x-c}+\frac{1}{d-x}\right)} & \text{for } c < x < d, \text{ and} \\ 0 & \text{else.} \end{cases} \tag{8.23}$$

If $\varphi(x)$ is a "good" test functen, then

$$x^\alpha P_n(x)\varphi(x) \tag{8.24}$$

[3] Laurent Schwartz. *Introduction to the Theory of Distributions*. University of Toronto Press, Toronto, 1952. collected and written by Israel Halperin

with any Polynomial $P_n(x)$, and in particular $x^n\varphi(x)$ also is a "good" test function.

Equipped with "good" test functions which have a finite support and are infinitely often differentiable, we can now give meaning to the transference 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 φ, we obtain

$$\begin{aligned} F'(\varphi) &:= \int_{-\infty}^{\infty}\left(\frac{d}{dx}q(x)\right)\varphi(x)dx \\ &= q(x)\varphi(x)\Big|_{x=-\infty}^{\infty} - \int_{-\infty}^{\infty} q(x)\left(\frac{d}{dx}\varphi(x)\right)dx \\ &= -\int_{-\infty}^{\infty} q(x)\left(\frac{d}{dx}\varphi(x)\right)dx \\ &= -F(\varphi'). \end{aligned} \tag{8.25}$$

By induction we obtain

$$F^{(n)}(\varphi) = \int_{-\infty}^{\infty}\left(\frac{d^n}{dx^n}q(x)\right)\varphi(x)dx = (-1)^n F(\varphi^{(n)}) = F((-1)^n\varphi^{(n)}). \tag{8.26}$$

8.1 Heaviside step function

One of the possible definitions of the Heaviside step function $H(x)$, and maybe the most common one – they differ in the value $H(0)$of at the origin $x = 0$, a difference which is irrelevant measure theoretically for "good" functions since it is only about an isolated point – is

$$H(x - x_0) = \begin{cases} 1 & \text{for } x \geq x_0 \\ 0 & \text{for } x < x_0 \end{cases} \tag{8.27}$$

It is plotted in Fig. 8.4.

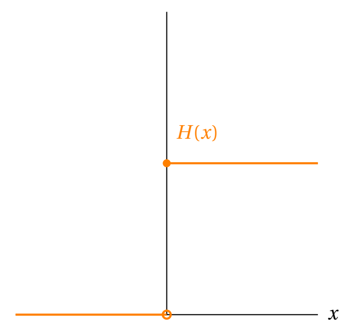


Figure 8.4: Plot of the Heaviside step function $H(x)$.

It is also very common to define the Heaviside step function as the *integral of the δ function*; likewise the delta function is the derivative of the Heaviside step function; that is,

$$\begin{aligned} H(x - x_0) &= \int_{-\infty}^{x-x_0}\delta(t)dt, \\ \frac{d}{dx}H(x-x_0) &= \delta(x-x_0). \end{aligned} \tag{8.28}$$

In the spirit of the above definition, it might have been more appropriate to define $H(0) = \frac{1}{2}$; that is,

$$H(x - x_0) = \begin{cases} 1 & \text{for } x > x_0 \\ \frac{1}{2} & \text{for } x = x_0 \\ 0 & \text{for } x < x_0 \end{cases} \tag{8.29}$$

and, since this affects only an isolated point at $x = 0$, we may happily do so if we prefer.

The latter equation can – in the sense of functionals – be proved through integration by parts as follows. Take

$$\begin{aligned}
&\int_{-\infty}^{\infty}\left[\frac{d}{dx}H(x-x_0)\right]\varphi(x)\,dx\\
&= H(x-x_0)\varphi(x)\Big|_{-\infty}^{\infty}-\int_{-\infty}^{\infty}H(x-x_0)\left[\frac{d}{dx}\varphi(x)\right]dx\\
&= H(-\infty)\varphi(-\infty)-\varphi(+\infty)-\int_{x_0}^{\infty}\left[\frac{d}{dx}\varphi(x)\right]dx\\
&= -\int_{x_0}^{\infty}\left[\frac{d}{dx}\varphi(x)\right]dx\\
&= -\,\varphi(x)\Big|_{x_0}^{\infty}\\
&= -[\varphi(\infty)-\varphi(x_0)]\\
&= \varphi(x_0).
\end{aligned} \tag{8.30}$$

Some other formulae involving the Heaviside step function are

$$H(\pm x)=\lim_{\epsilon\to 0^+}\frac{\mp i}{2\pi}\int_{-\infty}^{+\infty}\frac{e^{ikx}}{k\mp i\epsilon}dk, \tag{8.31}$$

and

$$H(x)=\frac{1}{2}+\sum_{l=0}^{\infty}(-1)^l\frac{(2l)!(4l+3)}{2^{2l+2}l!(l+1)!}P_{2l+1}(x), \tag{8.32}$$

where $P_{2l+1}(x)$ is a Legendre polynomial. Furthermore,

$$\delta(x)=\lim_{\epsilon\to 0}\frac{1}{\epsilon}H\left(\frac{\epsilon}{2}-|x|\right). \tag{8.33}$$

An integral representation of $H(x)$ is

$$H(x)=\lim\epsilon\downarrow 0^+\mp\frac{1}{2\pi i}\int_{-\infty}^{\infty}\frac{1}{t\pm i\epsilon}e^{\mp ixt}dt. \tag{8.34}$$

One commonly used limit form of the Heaviside step function is

$$H(x)=\lim_{\epsilon\to 0}H_\epsilon(x)=\lim_{\epsilon\to 0}\frac{1}{\pi x}\left[\frac{\pi}{2}+\tan^{-1}\frac{x}{\epsilon}\right]. \tag{8.35}$$

respectively.

Another limit representation is by a variant of the *sine integral function* $\text{Si}(x)=\int_0^x(\sin t)/t\,dt$ as follows [4]

$$\begin{aligned}
H(x)&=\lim_{t\to\infty}H_t(x)\\
&=\lim_{n\to\infty}\frac{2}{\pi}\int_0^n\frac{\sin(kx)}{x}dx\\
&=\frac{2}{\pi}\int_0^\infty\frac{\sin(kx)}{x}dx.
\end{aligned} \tag{8.36}$$

[4] Eli Maor. *Trigonometric Delights*. Princeton University Press, Princeton, 1998. URL http://press.princeton.edu/books/maor/

8.2 The sign function

The *sign function* is defined by

$$\text{sgn}(x-x_0)=\begin{cases}-1 & \text{for} x<x_0\\ 0 & \text{for} x=x_0\\ +1 & \text{for} x>x_0\end{cases}. \tag{8.37}$$

It is plotted in Fig. 8.5.

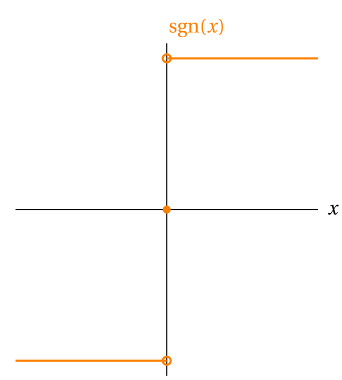


Figure 8.5: Plot of the sign function sgn(x).

In terms of the Heaviside step function it can be written by "stretching" the former by a factor of two, and shifting it for one negative unit as follows

$$\operatorname{sgn}(x-x_0) = 2H(x-x_0) - 1,$$
$$H(x-x_0) = \frac{1}{2}\left[\operatorname{sgn}(x-x_0)+1\right];\text{ and also}\operatorname{sgn}(x-x_0) = H(x-x_0) - H(x_0-x). \tag{8.38}$$

Note that

$$\operatorname{sgn}(x) = \frac{4}{\pi}\sum_{n=0}^{\infty}\frac{\sin[(2n+1)x]}{(2n+1)} \tag{8.39}$$
$$= \frac{4}{\pi}\sum_{n=0}^{\infty}(-1)^n\frac{\cos[(2n+1)(x-\pi/2)]}{(2n+1)},\ -\pi < x < \pi. \tag{8.40}$$

8.3 *Useful formulæ involving δ*

$$\delta(x) = \lim_{\epsilon\to 0}\frac{1}{\pi}\frac{\epsilon}{x^2+\epsilon^2} \tag{8.41}$$

$$\delta(x) = \lim_{\epsilon\to 0_+}\frac{1}{2\pi i}\left(\frac{1}{x-i\epsilon}-\frac{1}{x+i\epsilon}\right) = \lim_{\epsilon\to 0}\frac{1}{\pi}\frac{\epsilon}{x^2+\epsilon^2} \tag{8.42}$$

$$\lim_{\epsilon\to 0}\frac{1}{x\pm i\epsilon} = \frac{P}{x}\mp i\pi\delta(x) \tag{8.43}$$

$$\delta(x) = \delta(-x) \tag{8.44}$$

$$\delta(x) = \lim_{\epsilon\to 0}\frac{\theta(x+\epsilon)-\theta(x)}{\epsilon} = \frac{d}{dx}\theta(x) \tag{8.45}$$

$$\varphi(x)\delta(x-x_0) = \varphi(x_0)\delta(x-x_0) \tag{8.46}$$

$$x\delta(x) = 0 \tag{8.47}$$

For $a \neq 0$,

$$\delta(ax) = \frac{1}{|a|}\delta(x) \tag{8.48}$$

For the sake of a proof, consider the case $a > 0$ first:

$$\begin{aligned}&\int_{-\infty}^{\infty}\delta(ax)\varphi(x)dx\\ &= \tfrac{1}{a}\int_{-\infty}^{\infty}\delta(y)\varphi(\tfrac{y}{a})dy\\ &= \tfrac{1}{a}\varphi(0);\end{aligned} \tag{8.49}$$

and now the case $a < 0$:

$$\begin{aligned}&\int_{-\infty}^{\infty}\delta(ax)\varphi(x)dx\\ &= \tfrac{1}{a}\int_{\infty}^{-\infty}\delta(y)\varphi(\tfrac{y}{a})dy - \tfrac{1}{a}\int_{-\infty}^{\infty}\delta(y)\varphi(\tfrac{y}{a})dy\\ &= -\tfrac{1}{a}\varphi(0);\end{aligned} \tag{8.50}$$

If there exists a simple singularity x_0 of $f(x)$ in the integration interval, then

$$\delta(f(x)) = \frac{1}{|f'(x_0)|}\delta(x-x_0). \tag{8.51}$$

More generally, if f has only simple roots and f' is nonzero there,

$$\delta(f(x)) = \sum_{x_i}\frac{\delta(x-x_i)}{|f'(x_i)|} \tag{8.52}$$

where the sum extends over all simple roots x_i in the integration interval. In particular,

$$\delta(x^2 - x_0^2) = \frac{1}{2|x_0|}[\delta(x - x_0) + \delta(x + x_0)] \tag{8.53}$$

For a proof, note that, since f has only simpleroots, 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. (8.48) we obtain Eq. (8.52).

$$\delta'(f(x)) = \sum_{i=0}^{N} \frac{f''(x_i)}{|f'(x_i)|^3}\delta(x - x_i) + \sum_{i=0}^{N} \frac{f'(x_i)}{|f'(x_i)|^3}\delta'(x - x_i) \tag{8.54}$$

$$|x|\delta(x^2) = \delta(x) \tag{8.55}$$

$$-x\delta'(x) = \delta(x) \tag{8.56}$$

$$\delta^{(m)}(x) = (-1)^m \delta^{(m)}(-x), \tag{8.57}$$

where the index $^{(m)}$ denotes m–fold differentiation;

$$x^{m+1}\delta^{(m)}(x) = 0, \tag{8.58}$$

where the index $^{(m)}$ denotes m–fold differentiation;

$$x^2\delta'(x) = 0 \tag{8.59}$$

$$\delta(x) = \frac{d^2}{dx^2}[x\theta(x)] \tag{8.60}$$

If $\delta^3(\vec{r}) = \delta(x)\delta(y)\delta(r)$ with $\vec{r} = (x, y, z)$, then

$$\delta^3(\vec{r}) = \delta(x)\delta(y)\delta(z) = -\frac{1}{4\pi}\Delta\frac{1}{r} \tag{8.61}$$

$$\delta^3(\vec{r}) = -\frac{1}{4\pi}(\Delta + k^2)\frac{e^{ikr}}{r} \tag{8.62}$$

$$\delta^3(\vec{r}) = -\frac{1}{4\pi}(\Delta + k^2)\frac{\cos kr}{r} \tag{8.63}$$

In quantum field theory, phase space integrals of the form

$$\frac{1}{2E} = \int dp^0\, \theta(p^0)\delta(p^2 - m^2) \tag{8.64}$$

if $E = (\vec{p}^2 + m^2)^{(1/2)}$ are exploited.

8.4 Fourier transforms of δ and H

If $\{f_x(x)\}$ 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 $\widetilde{f}$ of f can be defined by [5]

$$\widetilde{f}(k) = \lim_{n\rightarrow\infty} \int_{-\infty}^{\infty} f_n(x) e^{-ikx} dx. \tag{8.65}$$

Since e^{-ikx} is not a particularly "good" function, $\widetilde{f}$ needs not be an ordinary function [6].

The Fourier transform of the δ-function can be obtained by insertion into Eq. (7.6)

$$\begin{aligned}\widetilde{\delta}(k) &= \int_{-\infty}^{\infty} \delta(x) e^{-ikx} dx \\ &= e^{-i0k} \int_{-\infty}^{\infty} \delta(x) dx \\ &= 1.\end{aligned} \tag{8.66}$$

That is, the Fourier transform of the δ-function is just a constant. δ-spiked signals carry all frequencies in them.

The Fourier transform of the Heaviside step function can also be obtained by insertion into Eq. (7.6)

$$\begin{aligned}\widetilde{H}(k) &= \int_{-\infty}^{\infty} H(x) e^{-ikx} dx \\ &= \frac{1}{2}\left[\delta(k) - \frac{i}{\pi k}\right].\end{aligned} \tag{8.67}$$

A *caveat* first: the following proof should *not* be understood in the usual functional, but rather in a functional sense.

$$\begin{aligned}\widetilde{H}(k) &= \int_{-\infty}^{\infty} H(x) e^{-ikx} dx \\ &= \int_{0}^{\infty} e^{-ikx} dx; \\ \widetilde{H}(-k) &= \int_{-\infty}^{\infty} H(x) e^{+ikx} dx \\ &= \int_{0}^{\infty} H(x) e^{+ikx} dx \\ &\text{[variable transformation: } x \rightarrow -x\text{]} \\ &= -\int_{0}^{-\infty} e^{-ikx} dx \\ &= \int_{-\infty}^{0} e^{-ikx} dx.\end{aligned} \tag{8.68}$$

Now separate the even part E from the odd part O of H; that is, define

$$\begin{aligned}E(k) &= (H(k) + H(-k)) \\ &= \int_{-\infty}^{+\infty} e^{-ikx} dx, \\ O(k) &= (H(k) - H(-k)) \\ &= \int_{0}^{\infty} \left[e^{-ikx} - e^{+ikx}\right] dx, \\ &= -2i \int_{0}^{\infty} \sin(kx) dx, \\ H(k) &= \frac{1}{2}(E(k) + O(k)).\end{aligned} \tag{8.69}$$

The two integrals defining E and O do not converge. However, one may

[5] M. J. Lighthill. *Introduction to Fourier Analysis and Generalized Functions*. Cambridge University Press, Cambridge, 1958; and Kenneth B. Howell. *Principles of Fourier analysis*. Chapman & Hall/CRC, Boca Raton, London, New York, Washington, D.C., 2001

[6] 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

approximate them by cutting the integrals off at some large value L

$$\begin{aligned} E_L(k) &= \int_{-L}^{+L} e^{-ikx}\,dx, \\ &= -\frac{e^{-ikx}}{ik}\Big|_{x=-L}^{+L}, \\ &= -\frac{e^{-ikL}-e^{+ikL}}{ik}, \\ &= 2\frac{\sin(kL)}{k}, \text{ and} \\ O_L(k) &= -2i\int_0^L \sin(kx)\,dx \\ &= -2i\frac{\cos(kx)}{k}\Big|_{x=0}^{+L}, \\ &= 2i\frac{[1-\cos(kL)]}{k}, \\ &= 4i\frac{\sin^2(\frac{kL}{2})}{k}. \end{aligned} \tag{8.70}$$

Now observe that, interpreted as distribution, $E_L(k)$ is proportional to a delta sequence, rendering

$$\lim_{L\to\infty} E_L(k) = \frac{1}{2}\delta(k). \tag{8.71}$$

In the same intepretation, when integrating over a test function, one can show that

$$\lim_{L\to\infty} O_L(k) = -\frac{i}{\pi k}. \tag{8.72}$$

It is possible to derive this result directly from the linearity of the Fourier transform: since by Eq. (8.38) $H(x) = \frac{1}{2}\left[\text{sgn}(x)+1\right]$,

$$\begin{aligned} \widetilde{H}(k) &= \frac{1}{2}\left[\widetilde{\text{sgn}}(k)+\tilde{1}\right] \\ &= \frac{1}{2}\left[\frac{1}{i\pi k}+\delta(k)\right]. \end{aligned} \tag{8.73}$$

Let us compute some concrete examples related to distributions.

1. For a start, let us proof that

$$\lim_{\epsilon\to 0}\frac{\epsilon\sin^2\frac{x}{\epsilon}}{\pi x^2} = \delta(x). \tag{8.74}$$

As a hint, take $\int_{-\infty}^{+\infty}\frac{\sin^2 x}{x^2}dx = \pi$.

Let us proof this conjecture by integrating over a good test function φ

$$\begin{aligned} &\frac{1}{\pi}\lim_{\epsilon\to 0}\int_{-\infty}^{+\infty}\frac{\epsilon\sin^2(\frac{x}{\epsilon})}{x^2}\varphi(x)dx \\ &\quad[\text{variable substitution} y=\frac{x}{\epsilon}, \frac{dy}{dx}=\frac{1}{\epsilon}, dx=\epsilon dy] \\ &\quad= \frac{1}{\pi}\lim_{\epsilon\to 0}\int_{-\infty}^{+\infty}\varphi(\epsilon y)\frac{\epsilon^2\sin^2(y)}{\epsilon^2 y^2}dy \\ &\quad= \frac{1}{\pi}\varphi(0)\int_{-\infty}^{+\infty}\frac{\sin^2(y)}{y^2}dy \\ &\quad= \varphi(0). \end{aligned} \tag{8.75}$$

Hence we can identify

$$\lim_{\epsilon\to 0}\frac{\epsilon\sin^2\left(\frac{x}{\epsilon}\right)}{\pi x^2} = \delta(x). \tag{8.76}$$

2. In order to prove that $\frac{1}{\pi}\frac{ne^{-x^2}}{1+n^2x^2}$ is a δ-sequence we proceed again by integrating over a good test function φ, and with the hint that $\int\limits_{-\infty}^{+\infty} dx/(1+x^2)=\pi$ we obtain

$$\begin{aligned}
&\lim_{n\to\infty}\frac{1}{\pi}\int\limits_{-\infty}^{+\infty}\frac{ne^{-x^2}}{1+n^2x^2}\varphi(x)dx \\
&\qquad \left[\text{variable substitution}\, y=xn,\, x=\frac{y}{n},\, \frac{dy}{dx}=n,\, dx=\frac{dy}{n}\right] \\
&=\lim_{n\to\infty}\frac{1}{\pi}\int\limits_{-\infty}^{+\infty}\frac{ne^{-\left(\frac{y}{n}\right)^2}}{1+y^2}\varphi\left(\frac{y}{n}\right)\frac{dy}{n} \\
&=\frac{1}{\pi}\int\limits_{-\infty}^{+\infty}\lim_{n\to\infty}\left[e^{-\left(\frac{y}{n}\right)^2}\varphi\left(\frac{y}{n}\right)\right]\frac{1}{1+y^2}dy \\
&=\frac{1}{\pi}\int\limits_{-\infty}^{+\infty}\left[e^0\varphi(0)\right]\frac{1}{1+y^2}dy \\
&=\frac{\varphi(0)}{\pi}\int\limits_{-\infty}^{+\infty}\frac{1}{1+y^2}dy \\
&=\frac{\varphi(0)}{\pi}\pi \\
&=\varphi(0)\,.
\end{aligned} \tag{8.77}$$

Hence we can identify

$$\lim_{n\to\infty}\frac{1}{\pi}\frac{ne^{-x^2}}{1+n^2x^2}=\delta(x). \tag{8.78}$$

3. Let us proof that $x^n\delta^{(n)}(x)=C\delta(x)$ and determine the constant C. We proceed again by integrating over a good test function φ. First note that if $\varphi(x)$ is a good test function, then so is $x^n\varphi(x)$.

$$\begin{aligned}
\int dx x^n\delta^{(n)}(x)\varphi(x) &= \int dx\delta^{(n)}(x)\left[x^n\varphi(x)\right]= \\
&= (-1)^n\int dx\delta(x)\left[x^n\varphi(x)\right]^{(n)}= \\
&= (-1)^n\int dx\delta(x)\left[nx^{n-1}\varphi(x)+x^n\varphi'(x)\right]^{(n-1)}= \\
&\dots \\
&= (-1)^n\int dx\delta(x)\left[\sum_{k=0}^{n}\begin{pmatrix}n\\k\end{pmatrix}(x^n)^{(k)}\varphi^{(n-k)}(x)\right]= \\
&= (-1)^n\int dx\delta(x)\left[n!\varphi(x)+n\cdot n!x\varphi'(x)+\cdots+x^n\varphi^{(n)}(x)\right]= \\
&= (-1)^n n!\int dx\delta(x)\varphi(x);
\end{aligned}$$

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. (8.52) 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

$$|f'(a)| = 2|a|, \qquad |f'(-a)| = |-2a| = 2|a|.$$

As a result,

$$\delta(x^2 - a^2) = \delta\big((x-a)(x+a)\big) = \frac{1}{|2a|}\big(\delta(x-a) + \delta(x+a)\big).$$

Taking this into account we finally obtain

$$\begin{aligned} &\int_{-\infty}^{+\infty} \delta(x^2 - a^2) g(x)\, dx \\ &= \int_{-\infty}^{+\infty} \frac{\delta(x-a)+\delta(x+a)}{2|a|} g(x)\, dx \\ &= \frac{g(a)+g(-a)}{2|a|}. \end{aligned} \tag{8.79}$$

5. Let us evaluate

$$I = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \delta(x_1^2 + x_2^2 + x_3^2 - R^2)\, d^3x \tag{8.80}$$

for $R \in \mathbb{R}, R > 0$. We may, of course, remain tn the standard ccartesian 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

$$I = \int_{r,\Omega} r^2 \delta(r^2 - R^2)\, d\Omega\, dr. \tag{8.81}$$

As the integral kernel $\delta(r^2 - R^2)$ just depends on the radial coordinate r the angular coordinates just integrate to 4π. Next we make use of Eq. (8.52), eliminate the solution for $r = -R$, and obtain

$$\begin{aligned} I &= 4\pi \int_0^\infty r^2 \delta(r^2 - R^2)\, dr \\ &= 4\pi \int_0^\infty r^2 \frac{\delta(r+R)+\delta(r-R)}{2R}\, dr \\ &= 4\pi \int_0^\infty r^2 \frac{\delta(r-R)}{2R}\, dr \\ &= 2\pi R. \end{aligned} \tag{8.82}$$

6. Let us compute

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \delta(x^3 - y^2 + 2y)\delta(x+y) H(y - x - 6) f(x,y)\, dx\, dy. \tag{8.83}$$

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. (8.52)

$$\delta(f(x)) = \sum_i \frac{1}{|f'(x_i)|}\delta(x - x_i),$$

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 δ-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 derivativs 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

$$\left(\frac{d}{dx} - \omega\right) H(x) e^{\omega x} \tag{8.84}$$

   as follows

$$\begin{aligned} &\tfrac{d}{dx}\left[H(x)e^{\omega x}\right] - \omega H(x) e^{\omega x} \\ &= \delta(x) e^{\omega x} + \omega H(x) e^{\omega x} - \omega H(x) e^{\omega x} \\ &= \delta(x) e^{0} \\ &= \delta(x) \end{aligned} \tag{8.85}$$

8. Next, simplify

$$\left(\frac{d^2}{dx^2} + \omega^2\right) \frac{1}{\omega} H(x) \sin(\omega x) \tag{8.86}$$

   as follows

$$\begin{aligned} &\tfrac{d^2}{dx^2}\left[\tfrac{1}{\omega} H(x) \sin(\omega x)\right] + \omega H(x) \sin(\omega x) \\ &= \tfrac{1}{\omega} \tfrac{d}{dx}\Big[\underbrace{\delta(x) \sin(\omega x)}_{=0} + \omega H(x) \cos(\omega x)\Big] + \omega H(x) \sin(\omega x) \\ &= \tfrac{1}{\omega}\Big[\omega \underbrace{\delta(x) \cos(\omega x)}_{\delta(x)} - \omega^2 H(x) \sin(\omega x)\Big] + \omega H(x) \sin(\omega x) = \delta(x) \end{aligned} \tag{8.87}$$

9. Let us compute the nth derivative of

$$f(x)=\begin{cases}0, & \text{für } x<0;\\ x, & \text{für } 0\le x\le 1;\\ 0, & \text{für } x>1.\end{cases} \tag{8.88}$$

As depicted in Fig. 8.6, 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)

$$\begin{aligned} f(x) &= x\left[H(x)-H(x-1)\right]=xH(x)-xH(x-1)\\ f'(x) &= H(x)+x\delta(x)-H(x-1)-x\delta(x-1)\end{aligned}$$

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)

$$\begin{aligned} f(x) &= xH(x)H(1-x)\\ f'(x) &= H(x)H(1-x)+\underbrace{x\delta(x)}_{=0}H(1-x)+\underbrace{xH(x)(-1)\delta(1-x)}_{-H(x)\delta(1-x)}=\\ &= H(x)H(1-x)-\delta(1-x)=[\delta(x)=\delta(-x)]=H(x)H(1-x)-\delta(x-1)\\ f''(x) &= \underbrace{\delta(x)H(1-x)}_{=\delta(x)}+\underbrace{(-1)H(x)\delta(1-x)}_{-\delta(1-x)}-\delta'(x-1)=\\ &= \delta(x)-\delta(x-1)-\delta'(x-1)\end{aligned}$$

and hence by induction

$$f^{(n)}(x)=\delta^{(n-2)}(x)-\delta^{(n-2)}(x-1)-\delta^{(n-1)}(x-1)$$

for $n>1$.

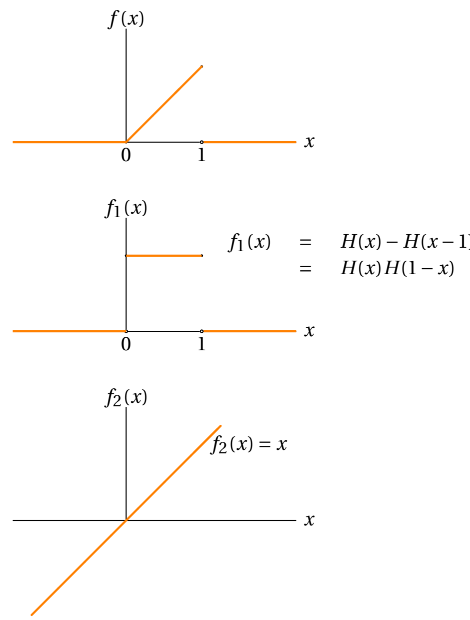


Figure 8.6: Composition of $f(x)$

10. Let us compute the nth derivative of

$$f(x)=\begin{cases}|\sin x|, & \text{for } -\pi\le x\le \pi;\\ 0, & \text{for } |x|>\pi.\end{cases} \tag{8.89}$$

$$f(x)=|\sin x|H(\pi+x)H(\pi-x)$$

$$|\sin x|=\sin x\,\mathrm{sgn}(\sin x)=\sin x\,\mathrm{sgn}\,x \qquad \text{für} \quad -\pi<x<\pi;$$

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

$$\begin{aligned}
f^{(n)} &= f^{(n-4)}(x) - 2\delta^{(n-4)}(x) + 2\delta^{(n-2)}(x) - \delta^{(n-4)}(\pi + x) +\\
&\quad + \delta^{(n-2)}(\pi + x) + (-1)^{n-1}\delta^{(n-4)}(\pi - x) + (-1)^n\delta^{(n-2)}(\pi - x)\\
&\quad (n = 4, 5, 6, \dots)
\end{aligned}$$

9
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, $[y(x)]^2$.

9.1 Elegant way to solve linear differential equations

Green's function present a very elegant way of solving linear differential equations of the form

$$\begin{aligned} &\mathscr{L}_x y(x) = f(x), \text{ with the differential operator} \\ &\mathscr{L}_x = a_n(x)\frac{d^n}{dx^n} + a_{n-1}(x)\frac{d^{n-1}}{dx^{n-1}} + \ldots + a_1(x)\frac{d}{dx} + a_0(x) \\ &\quad = \sum_{j=0}^{n} a_j(x)\frac{d^j}{dx^j}, \end{aligned} \tag{9.1}$$

where $a_i(x)$, $0 \le i \le n$ are functions of x. The idea is quite straightforward: if we are able to obtain the "inverse" G of the differential operator $\mathscr{L}$ defined by

$$\mathscr{L}_x G(x,x') = \delta(x-x'), \tag{9.2}$$

with δ representing Dirac's delta function, then the solution to the inhomogenuous differential equation (9.1) can be obtained by integrating $G(x-x')$ alongside with the inhomogenuous term $f(x')$; that is,

$$y(x) = \int_{-\infty}^{\infty} G(x,x')f(x')dx'. \tag{9.3}$$

This claim, as posted in Eq. (9.3), can be verified by explicitly applying the differential operator $\mathscr{L}_x$ to the solution $y(x)$,

$$\begin{aligned} &\mathscr{L}_x y(x) \\ &\quad = \mathscr{L}_x \int_{-\infty}^{\infty} G(x,x')f(x')dx' \\ &\quad = \int_{-\infty}^{\infty} \mathscr{L}_x G(x-x')f(x')dx' \\ &\quad = \int_{-\infty}^{\infty} \delta(x-x')f(x')dx' \\ &\quad = f(x). \end{aligned} \tag{9.4}$$

Let us check whether $G(x,x') = \theta(x-x')\sinh(x-x')$ is a Green's function of the differential operator $\mathscr{L}_x = \frac{d^2}{dx^2} - 1$. In this case, all we have to do is to verify that $\mathscr{L}_x$, applied to $G(x,x')$, actually renders $\delta(x-x')$, as required by Eq. (9.2).

$$\begin{aligned}\mathscr{L}_x G(x,x') &= \delta(x-x') \\ \left(\frac{d^2}{dx^2} - 1\right)\Theta(x-x')\sinh(x-x') &\overset{?}{=} \delta(x-x')\end{aligned}$$

Note that $\dfrac{d}{dx}\sinh x = \cosh x$, $\quad \dfrac{d}{dx}\cosh x = \sinh x$; and hence

$$\frac{d}{dx}\left(\underbrace{\delta(x-x')\sinh(x-x')}_{=0} + \Theta(x-x')\cosh(x-x')\right) - \Theta(x-x')\sinh(x-x') =$$

$$\delta(x-x')\cosh(x-x') + \Theta(x-x')\sinh(x-x') - \Theta(x-x')\sinh(x-x') = \delta(x-x').$$

The solution (9.4) so obtained is *not unique*, as it is only a special solution to the inhomogenuous equation (9.1).

Note that the general solution to (9.1) can be found by adding the general solution $y_0(x)$ of the corresponding *homogenuous* differential equation

$$\mathscr{L}_x y(x) = 0 \tag{9.5}$$

to one special solution – say, the one obtained in Eq. (9.4) through Green's function techniques.

Indeed, the most general solution

$$Y(x) = y(x) + y_0(x) \tag{9.6}$$

clearly is a solution of the inhomogenuous differential equation (9.4), as

$$\mathscr{L}_x Y(x) = \mathscr{L}_x y(x) + \mathscr{L}_x y_0(x) = f(x) + 0 = f(x). \tag{9.7}$$

Conversely, any two distinct special solutions $y_1(x)$ and $y_2(x)$ of the inhomogenuous differential equation (9.4) differ only by a function which is a solution tho the homogenuous differential equation (9.5), because due to linearity of $\mathscr{L}_x$, their difference $y_d(x) = y_1(x) - y_2(x)$ can be parameterized by some function in y_0

$$\mathscr{L}_x[y_1(x) - y_2(x)] = \mathscr{L}_x y_1(x) + \mathscr{L}_x y_2(x) = f(x) - f(x) = 0. \tag{9.8}$$

From now on, we assume that the coefficients $a_j(x) = a_j$ in Eq. (9.1) are constants, and thus *translational invariant*. Then the entire *Ansatz* (9.2) 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,

$$G(x,x') = G(x-x'). \tag{9.9}$$

For such translation invariant systems, the Fourier analysis represents an excellent way of analyzing the situation.

Let us see why translanslation invariance of the coefficients $a_j(x) = a_j(x+\xi) = a_j$ under the translation $x \to x+\xi$ with arbitrary ξ – 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. Translanslation invariance of the Green's function really means

$$G(x+\xi, x'+\xi) = G(x, x'). \tag{9.10}$$

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

$$G(x-x', x'-x') = G(x-x', 0) \to G(x-x'). \tag{9.11}$$

What is important for applications is the possibility to adapt the solutions of some inhomogenuous 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, $i = 1, \ldots, k$. Then, the Green's function G must vanish there also

$$G(x_i - x') = 0 \text{ for } i = 1, \ldots, k. \tag{9.12}$$

9.2 *Finding Green's functions by spectral decompositions*

Suppose $\psi_i(x)$ are *eigenfunctions* of the differential operator $\mathcal{L}_x$, and λ_i are the associated *eigenvalues*; that is,

$$\mathcal{L}_x \psi_i(x) = \lambda_i \psi_i(x). \tag{9.13}$$

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 $\psi_1(x), \psi_2(x), \ldots, \psi_n(x)$ of $\mathcal{L}_x$. In this case, orthogonality of the system of eigenfunctions holds, such that

$$\sum_{i=1}^{n} \psi_i(x)\overline{\psi_i(x')} = \delta(x-x'). \tag{9.14}$$

$\overline{\psi_i(x')}$ stands for the complex conjugate of $\psi_i(x')$. The sum in Eq. (9.14) stands for an integral in the case of contiuous spectrum of $\mathcal{L}_x$.

Take, for instance the differential equation corresponding to the harmonic oscillator

$$\mathcal{L}_t = \frac{d^2}{dt^2} + k^2, \tag{9.15}$$

with $\omega \in \mathbb{R}$. Then the associated eigenfunctions are

$$\psi_k(t) = e^{-ikt}, \tag{9.16}$$

with $\infty \le k \le \infty$. Taking the complex conjugate and integration over k yields

$$\begin{aligned}
&\int_{-\infty}^{\infty} \psi_k(t)\overline{\psi_k(t')}dk \\
&\quad = \int_{-\infty}^{\infty} e^{-ikt}e^{ikt'}dk \\
&\quad = \int_{-\infty}^{\infty} e^{-ik(t-t')}dk \\
&\quad = \delta(t-t').
\end{aligned} \tag{9.17}$$

Then the Green's function of $\mathscr{L}_x$ can be written as the spectral sum of the absolute squares of the eigenfunctions, devided by the eigenvalues λ_j; that is,

$$G(x-x') = \sum_{j=1}^{n} \frac{\psi_j(x)\overline{\psi_j(x')}}{\lambda_j}. \tag{9.18}$$

For the sake of proof, apply the differential operator $\mathscr{L}_x$ to the Greens function *Ansatz* G of Eq. (9.18) and verify that it satisfies Eq. (9.2):

$$\begin{aligned}
&\mathscr{L}_x G(x-x') \\
&\quad = \mathscr{L}_x \sum_{j=1}^{n} \frac{\psi_j(x)\overline{\psi_j(x')}}{\lambda_j} \\
&\quad = \sum_{j=1}^{n} \frac{[\mathscr{L}_x \psi_j(x)]\overline{\psi_j(x')}}{\lambda_j} \\
&\quad = \sum_{j=1}^{n} \frac{[\lambda_j \psi_j(x)]\overline{\psi_j(x')}}{\lambda_j} \\
&\quad = \sum_{j=1}^{n} \psi_j(x)]\overline{\psi_j(x')} \\
&\quad = \delta(x-x').
\end{aligned} \tag{9.19}$$

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

$$\mathscr{L}_x y(x) = \frac{d^4}{dx^4} y(x) = q(x) \approx c, \tag{9.20}$$

with constant $c \in \mathbb{R}$. Let us further assume the boundary conditions

$$y(0) = y(L) = \frac{d^2}{dx^2} y(0) = \frac{d^2}{dx^2} y(L) = 0. \tag{9.21}$$

Also, we require that $y(\text{x})$ 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 $\mathscr{L}_x$ can be written as

$$\psi_j(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{\pi j x}{L}\right) \tag{9.22}$$

for $j = 1, 2, \ldots$. The associated eigenvalues

$$\lambda_j = \left(\frac{\pi j}{L}\right)^4$$

can be verified through explicit differentiation

$$
\begin{aligned}
\mathcal{L}_x\psi_j(x) &= \mathcal{L}_x\sqrt{\tfrac{2}{L}}\sin\left(\tfrac{\pi j x}{L}\right)\\
&= \mathcal{L}_x\sqrt{\tfrac{2}{L}}\sin\left(\tfrac{\pi j x}{L}\right)\\
&= \left(\tfrac{\pi j}{L}\right)^4\sqrt{\tfrac{2}{L}}\sin\left(\tfrac{\pi j x}{L}\right)\\
&= \left(\tfrac{\pi j}{L}\right)^4\psi_j(x).
\end{aligned}
\tag{9.23}
$$

The cosine functions which are also solutions of the Euler-Bernoulli equations (9.20) do not vanish at the origin $x = 0$.

Hence,

$$
\begin{aligned}
G(x-x')(x) &= \tfrac{2}{L}\sum_{j=1}^{\infty}\frac{\sin\left(\frac{\pi j x}{L}\right)\sin\left(\frac{\pi j x'}{L}\right)}{\left(\frac{\pi j}{L}\right)^4}\\
&= \tfrac{2L^3}{\pi^4}\sum_{j=1}^{\infty}\tfrac{1}{j^4}\sin\left(\tfrac{\pi j x}{L}\right)\sin\left(\tfrac{\pi j x'}{L}\right)
\end{aligned}
\tag{9.24}
$$

Finally we are in a good shape to calculate the solution explicitly by

$$
\begin{aligned}
y(x) &= \int_0^L G(x-x')g(x')dx'\\
&\approx \int_0^L c\left[\tfrac{2L^3}{\pi^4}\sum_{j=1}^{\infty}\tfrac{1}{j^4}\sin\left(\tfrac{\pi j x}{L}\right)\sin\left(\tfrac{\pi j x'}{L}\right)\right]dx'\\
&\approx \tfrac{2cL^3}{\pi^4}\sum_{j=1}^{\infty}\tfrac{1}{j^4}\sin\left(\tfrac{\pi j x}{L}\right)\left[\int_0^L\sin\left(\tfrac{\pi j x'}{L}\right)dx'\right]\\
&\approx \tfrac{4cL^4}{\pi^5}\sum_{j=1}^{\infty}\tfrac{1}{j^5}\sin\left(\tfrac{\pi j x}{L}\right)\sin^2\left(\tfrac{\pi j}{2}\right)
\end{aligned}
\tag{9.25}
$$

9.3 *Finding Green's functions by Fourier analysis*

If one is dealing with translation invariant systems of the form

$$
\begin{aligned}
&\mathcal{L}_x y(x) = f(x), \text{ with the differential operator}\\
&\mathcal{L}_x = a_n\tfrac{d^n}{dx^n} + a_{n-1}\tfrac{d^{n-1}}{dx^{n-1}} + \ldots + a_1\tfrac{d}{dx} + a_0\\
&\quad = \sum_{j=0}^{n} a_j(x)\tfrac{d^j}{dx^j},
\end{aligned}
\tag{9.26}
$$

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. (8.66) on page 135 the Fourier transform of the delta function $\widetilde{\delta}(k) = 1$ is just a constant; with our definition unity. Then, δ can be written as

$$
\delta(x-x') = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{ik(x-x')}dk \tag{9.27}
$$

Next, consider the Fourier transform of the Green's function

$$
\widetilde{G}(k) = \int_{-\infty}^{\infty} G(x)e^{-ikx}dx \tag{9.28}
$$

and its back trasform

$$
G(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty}\widetilde{G}(k)e^{ikx}dk. \tag{9.29}
$$

Insertion of Eq. (9.29) into the *Ansatz* $\mathcal{L}_x G(x-x') = \delta(x-x')$ yields

$$
\begin{aligned}
&\mathcal{L}_x G(x)\\
&\quad = \mathcal{L}_x\tfrac{1}{2\pi}\int_{-\infty}^{\infty}\widetilde{G}(k)e^{ikx}dk\\
&\quad = \tfrac{1}{2\pi}\int_{-\infty}^{\infty}\widetilde{G}(k)\left(\mathcal{L}_x e^{ikx}\right)dk = \tfrac{1}{2\pi}\int_{-\infty}^{\infty}e^{ikx}dk.
\end{aligned}
\tag{9.30}
$$

and thus, through comparison of the integral kernels,

$$\begin{aligned} &\frac{1}{2\pi}\int_{-\infty}^{\infty}\left[\widetilde{G}(k)\mathscr{L}_x - 1\right]e^{ikx}dk = 0,\\ &\widetilde{G}(k)\mathscr{L}_k - 1 = 0, \\ &\widetilde{G}(k) = (\mathscr{L}_k)^{-1}, \end{aligned} \tag{9.31}$$

where $\mathscr{L}_k$ is obtained from $\mathscr{L}_x$ by substituting every derivative $\frac{d}{dx}$ in the latter by ik in the former. in that way, the Fourier transform $\widetilde{G}(k)$ is obtained as a polynomial of degree n, the same degree as the highest order of derivative in $\mathscr{L}_x$.

In order to obtain the Green's function $G(x)$, and to be able to integrate over it with the inhomogenuous term $f(x)$, we have to Fourier transform $\widetilde{G}(k)$ 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 homogenuos equation $\mathscr{L}_x G(x-x') = 0$. 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 intervall $[0,\infty)$ with the boundary conditions $y(0) = 0$.

   We observe that the associated differential operator is given by

   $$\mathscr{L}_t = \frac{d}{dt} - 1,$$

   and the inhomogenuous term can be identified with $f(t) = t$.

   We use the *Ansatz* $G_1(t,t') = \frac{1}{2\pi}\int\limits_{-\infty}^{+\infty}\tilde{G}_1(k)e^{ik(t-t')}dk$; hence

   $$\begin{aligned} \mathscr{L}_t G_1(t,t') &= \frac{1}{2\pi}\int\limits_{-\infty}^{+\infty}\tilde{G}_1(k)\underbrace{\left(\frac{d}{dt}-1\right)e^{ik(t-t')}}_{=(ik-1)e^{ik(t-t')}}dk = \\ &= \delta(t-t') = \frac{1}{2\pi}\int\limits_{-\infty}^{+\infty}e^{ik(t-t')}dk \end{aligned}$$

   Now compare the kernels of the Fourier integrals of $\mathscr{L}_t G_1$ and δ:

   $$\tilde{G}_1(k)(ik-1) = 1 \Longrightarrow \tilde{G}_1(k) = \frac{1}{ik-1} = \frac{1}{i(k+i)}$$

   $$G_1(t,t') = \frac{1}{2\pi}\int\limits_{-\infty}^{+\infty}\frac{e^{ik(t-t')}}{i(k+i)}dk$$

   The paths in the upper and lower integration plain are drawn in Frig. 9.1.

   The "closures" throught the respective half-circle paths vanish.

   $$\text{residuum theorem: } G_1(t,t') \quad = \quad 0 \qquad \text{for} \quad t > t'$$

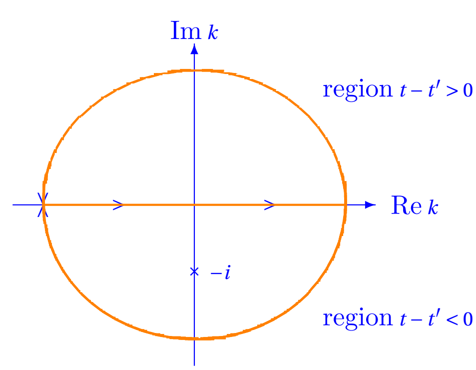


Figure 9.1: Plot of the two paths reqired for solving the Fourier integral.

$$
\begin{aligned}
G_1(t,t') &= -2\pi i \,\text{Res}\left(\frac{1}{2\pi i}\frac{e^{ik(t-t')}}{(k+i)};-i\right) = \\
&= -e^{t-t'} \quad \text{for } t<t'.
\end{aligned}
$$

Hence we obtain a Green's function for the inhomogenuous differential equation

$$G_1(t,t') = -\Theta(t'-t)e^{t-t'}$$

However, this Green's function and its associated (special) solution does not obey the boundary conditions $G_1(0,t') = -\Theta(t')e^{-t'} \neq 0$ for $t' \in [0,\infty)$.

Therefore, we have to fit the Greens function by adding an appropriately weighted solution to the homogenuos differential equation. The homogenuous Green's function is found by

$$\mathscr{L}_t G_0(t,t') = 0,$$

and thus, in particular,

$$\frac{d}{dt}G_0 = G_0 \Longrightarrow G_0 = ae^{t-t'}.$$

with the *Ansatz*

$$G(0,t') = G_1(0,t') + G_0(0,t';a) = -\Theta(t')e^{-t'} + ae^{-t'}$$

for the general solution we can choose the constant coefficient a so that

$$G(0,t') = G_1(0,t') + G_0(0,t';a) = -\Theta(t')e^{-t'} + ae^{-t'} = 0$$

For $a=1$, the Green's function and thus the solution obeys the boundary value conditions; that is,

$$G(t,t') = \left[1-\Theta(t'-t)\right]e^{t-t'}.$$

Since $\Theta(-x) = 1-\Theta(x)$, $G(t,t')$ can be rewritten as

$$G(t,t') = \Theta(t-t')e^{t-t'}.$$

In the final step we obtain the solution through integration of G over the inhomogenuous term t:

$$
\begin{aligned}
y(t) &= \int_0^\infty \underbrace{\Theta(t-t')}_{=1 \text{ for } t'<t} e^{t-t'}t'dt' = \\
&= \int_0^t e^{t-t'}t'dt' = e^t\int_0^t t'e^{-t'}dt' = \\
&= e^t\left(-t'e^{-t'}\Big|_0^t - \int_0^t(-e^{-t'})dt'\right) = \\
&= e^t\left[(-te^{-t}) - e^{-t'}\Big|_0^t\right] = e^t\left(-te^{-t} - e^{-t} + 1\right) = e^t - 1 - t.
\end{aligned}
$$

2. Next, let us solve the differential equation $\frac{d^2y}{dt^2} + y = \cos t$ on the intervall $t \in [0,\infty)$ with the boundary conditions $y(0) = y'(0) = 0$.

   First, observe that
$$\mathscr{L} = \frac{d^2}{dt^2} + 1.$$
   The Fourier *Ansatz* for the Green's function is
$$\begin{aligned}
G_1(t,t') &= \frac{1}{2\pi}\int\limits_{-\infty}^{+\infty} \tilde{G}(k)e^{ik(t-t')}dk\\
\mathscr{L}G_1 &= \frac{1}{2\pi}\int\limits_{-\infty}^{+\infty} \tilde{G}(k)\left(\frac{d^2}{dt^2}+1\right)e^{ik(t-t')}dk =\\
&= \frac{1}{2\pi}\int\limits_{-\infty}^{+\infty} \tilde{G}(k)((ik)^2+1)e^{ik(t-t')}dk =\\
&= \delta(t-t') = \frac{1}{2\pi}\int\limits_{-\infty}^{+\infty} e^{ik(t-t')}dk =
\end{aligned}$$
   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
$$\begin{aligned}
G_1(t,t') &= -\frac{1}{2\pi}\int\limits_{-\infty}^{+\infty} \frac{e^{ik(t-t')}}{(k+1)(k-1)}dk =\\
&= -\frac{1}{2\pi}2\pi i\left[\text{Res}\left(\frac{e^{ik(t-t')}}{(k+1)(k-1)};k=1\right)+\right.\\
&\qquad \left.\text{Res}\left(\frac{e^{ik(t-t')}}{(k+1)(k-1)};k=-1\right)\right]\Theta(t-t')
\end{aligned}$$
   The path in the upper integration plain is drawn in Fig. 9.2.

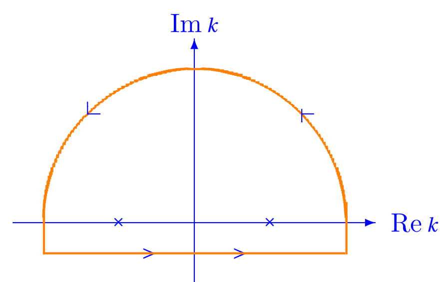


Figure 9.2: Plot of the path reqired for solving the Fourier integral.

$$\begin{aligned}
G_1(t,t') &= -\frac{i}{2}\left(e^{i(t-t')}-e^{-i(t-t')}\right)\Theta(t-t') =\\
&= \frac{e^{i(t-t')}-e^{-i(t-t')}}{2i}\Theta(t-t') = \sin(t-t')\Theta(t-t')\\
G_1(0,t') &= \sin(-t')\Theta(-t') = 0 \qquad \text{weil} \quad t'>0\\
G_1'(t,t') &= \cos(t-t')\Theta(t-t') + \underbrace{\sin(t-t')\delta(t-t')}_{=0}\\
G_1'(0,t') &= \cos(-t')\Theta(-t') = 0 \qquad \text{wie vorher}
\end{aligned}$$

G_1 already satisfies the boundary conditions; hence we do not need to find the Green's function G_0 of the homogenuous equation.

$$
\begin{aligned}
y(t) &= \int_0^\infty G(t,t')f(t')dt' = \int_0^\infty \sin(t-t') \underbrace{\Theta(t-t')}_{=1 \text{ for } t>t'} \cos t'dt' = \\
&= \int_0^t \sin(t-t')\cos t'dt' = \int_0^t (\sin t\cos t' - \cos t\sin t')\cos t'dt' = \\
&= \int_0^t \left[\sin t(\cos t')^2 - \cos t\sin t'\cos t'\right]dt' = \\
&= \sin t\int_0^t (\cos t')^2 dt' - \cos t\int_0^t sint'\cos t'dt' = \\
&= \sin t\left[\frac{1}{2}(t'+\sin t'\cos t')\right]\Big|_0^t - \cos t\left[\frac{\sin^2 t'}{2}\right]\Big|_0^t = \\
&= \frac{t\sin t}{2} + \frac{\sin^2 t\cos t}{2} - \frac{\cos t\sin^2 t}{2} = \frac{t\sin t}{2}.
\end{aligned}
$$

Part IV:
Differential equations

10
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 [1]. In physics, many formalizations involve second order differential equations, which, in their most general form, can be written as [2]

$$\mathcal{L}_x y(x) = a_0(x)y(x) + a_1(x)\frac{d}{dx}y(x) + a_2(x)\frac{d^2}{dx^2}y(x) = f(x). \tag{10.1}$$

The differential operator is defined by

$$\mathcal{L}_x y(x) = a_0(x) + a_1(x)\frac{d}{dx} + a_2(x)\frac{d^2}{dx^2}. \tag{10.2}$$

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.

[1] 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 *Sturm-Liouville Theory, Past and Present*, pages 271–331. Birkhäuser Verlag, Basel, 2005. URL http://www.math.niu.edu/SL2/papers/birk0.pdf

[2] 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. Creative Commons Attribution-NoncommercialShare Alike 3.0 United States License

10.1 Sturm-Liouville form

Any second order differential equation of the general form (10.1) can be rewritten into a differential equation of the *Sturm-Liouville form*

$$\begin{aligned}
&\mathcal{S}_x y(x) = \frac{d}{dx}\left[p(x)\frac{d}{dx}\right]y(x) + q(x)y(x) = F(x), \text{ with}\\
&p(x) = e^{\int \frac{a_1(x)}{a_2(x)}dx},\\
&q(x) = p(x)\frac{a_0(x)}{a_2(x)} = \frac{a_0(x)}{a_2(x)}e^{\int \frac{a_1(x)}{a_2(x)}dx},\\
&F(x) = p(x)\frac{f(x)}{a_2(x)} = \frac{f(x)}{a_2(x)}e^{\int \frac{a_1(x)}{a_2(x)}dx},
\end{aligned} \tag{10.3}$$

The associated differential operator

$$\begin{aligned}
\mathcal{S}_x &= \frac{d}{dx}\left[p(x)\frac{d}{dx}\right] + q(x)\\
&= p(x)\frac{d^2}{dx^2} + p'(x)\frac{d}{dx} + q(x)
\end{aligned} \tag{10.4}$$

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. (10.3) and compare it with Eq. (10.1).

$$\begin{aligned}
&\left\{\frac{d}{dx}\left[e^{\int \frac{a_1(x)}{a_2(x)}dx}\frac{d}{dx}\right]+\frac{a_0(x)}{a_2(x)}e^{\int \frac{a_1(x)}{a_2(x)}dx}\right\}y(x)=\frac{f(x)}{a_2(x)}e^{\int \frac{a_1(x)}{a_2(x)}dx}\\
&e^{\int \frac{a_1(x)}{a_2(x)}dx}\left\{\frac{d^2}{dx^2}+\frac{a_1(x)}{a_2(x)}\frac{d}{dx}+\frac{a_0(x)}{a_2(x)}\right\}y(x)=\frac{f(x)}{a_2(x)}e^{\int \frac{a_1(x)}{a_2(x)}dx}\\
&\left\{a_2(x)\frac{d^2}{dx^2}+a_1(x)\frac{d}{dx}+a_0(x)\right\}y(x)=f(x).
\end{aligned} \tag{10.5}$$

10.2 Sturm-Liouville eigenvalue problem

The Sturm-Liouville eigenvalue problem is given by the differential equation

$$\begin{aligned}
&\mathscr{S}_x\phi(x)=\lambda\rho(x)\phi(x), \text{ or}\\
&\frac{d}{dx}\left[p(x)\frac{d}{dx}\right]\phi(x)+[q(x)-\lambda\rho(x)]\phi(x)=0
\end{aligned} \tag{10.6}$$

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. [3]) that

[3] M. A. Al-Gwaiz. *Sturm-Liouville Theory and its Applications*. Springer, London, 2008

- the eigenvalues λ turn out to be real, countable, and ordered, and that there is a smallest eigenvalue λ_1 such that $\lambda_1<\lambda_2<\lambda_2<\cdots$;

- for each eigenvalue λ_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,

$$\langle\phi_j\mid\phi_k\rangle=\int_a^b\phi_j(x)\phi_k(x)\rho(x)dx=\delta_{jk} \tag{10.7}$$

- the set of eigenfunctions is *complete*; that is, any piecewise smooth function can be represented by

$$\begin{aligned}
&f(x)=\sum_{k=1}^\infty c_k\phi_k(x),\\
&\text{with}\\
&c_k=\frac{\langle f\vert\phi_k(x)\rangle}{\langle\phi_k(x)\vert\phi_k(x)\rangle}.
\end{aligned} \tag{10.8}$$

- the orthonormal (with respect to the weight ρ) set $\{\phi_j(x)\mid j\in\mathbb{N}\}$ is a *basis* of a Hilbert space with the inner product

$$\langle f\mid g\rangle=\int_a^b f(x)g(x)\rho(x)dx. \tag{10.9}$$

10.3 *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. (10.9). In this formalization, the Sturm-Liouville differential operator $\mathcal{S}$ 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 φ satisfying boundary conditions.

$$\int_a^b |\varphi(x)|^2 \rho(x)\,dx < \infty. \tag{10.10}$$

Then, the adjoint operator $\mathcal{L}^\dagger$ is defined by satisfying

$$\begin{aligned} \langle \psi \mid \mathcal{L}\varphi\rangle &= \int_a^b \psi(x)[\mathcal{L}\varphi(x)]\rho(x)\,dx \\ &= \langle \mathcal{L}^\dagger\psi \mid \varphi\rangle = \int_a^b [\mathcal{L}^\dagger\psi(x)]\varphi(x)\rho(x)\,dx \end{aligned} \tag{10.11}$$

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 (10.2) and with $\rho(x) = 1$, we can move the differential quotients and the entire differential operator in

$$\begin{aligned} \langle \psi \mid \mathcal{L}\varphi\rangle &= \int_a^b \psi(x)[\mathcal{L}_x\varphi(x)]\rho(x)\,dx \\ &= \int_a^b \psi(x)[a_2(x)\varphi''(x) + a_1(x)\varphi'(x) + a_0(x)\varphi(x)]\,dx \end{aligned} \tag{10.12}$$

from φ to ψ by one and two partial integrations.

Integrating the kernel $a_1(x)\varphi'(x)$ by parts yields

$$\int_a^b \psi(x)a_1(x)\varphi'(x)\,dx = \psi(x)a_1(x)\varphi(x)\Big|_a^b - \int_a^b (\psi(x)a_1(x))'\varphi(x)\,dx. \tag{10.13}$$

Integrating the kernel $a_2(x)\varphi''(x)$ by parts twice yields

$$\begin{aligned} \int_a^b \psi(x)a_2(x)\varphi''(x)\,dx &= \psi(x)a_2(x)\varphi'(x)\Big|_a^b - \int_a^b (\psi(x)a_2(x))'\varphi'(x)\,dx \\ &= \psi(x)a_2(x)\varphi'(x)\Big|_a^b - (\psi(x)a_2(x))'\varphi(x)\Big|_a^b + \int_a^b (\psi(x)a_2(x))''\varphi(x)\,dx \\ &= \psi(x)a_2(x)\varphi'(x) - (\psi(x)a_2(x))'\varphi(x)\Big|_a^b + \int_a^b (\psi(x)a_2(x))''\varphi(x)\,dx. \end{aligned} \tag{10.14}$$

Combining these two calculations yields

$$\begin{aligned} \langle \psi \mid \mathcal{L}\varphi\rangle &= \int_a^b \psi(x)[\mathcal{L}_x\varphi(x)]\rho(x)\,dx \\ &= \int_a^b \psi(x)[a_2(x)\varphi''(x) + a_1(x)\varphi'(x) + a_0(x)\varphi(x)]\,dx \\ &= \psi(x)a_1(x)\varphi(x) + \psi(x)a_2(x)\varphi'(x) - (\psi(x)a_2(x))'\varphi(x)\Big|_a^b \\ &\quad + \int_a^b [(a_2(x)\psi(x))'' - (a_1(x)\psi(x))' + a_0(x)\psi(x)]\varphi(x)\,dx. \end{aligned} \tag{10.15}$$

If the terms with no integral vanish (because of boundary contitions 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. (10.15) reduces to

$$\langle \psi \mid \mathcal{L}\varphi\rangle = \int_a^b [(a_2(x)\psi(x))'' - (a_1(x)\psi(x))' + a_0(x)\psi(x)]\varphi(x)\,dx, \tag{10.16}$$

and we can identify the adjoint differential operator $\mathscr{L}_x$ with

$$\begin{aligned}\mathscr{L}_x^\dagger &= \frac{d^2}{dx^2}a_2(x) - \frac{d}{dx}a_1(x) + a_0(x)\\ &= \frac{d}{dx}\left[a_2(x)\frac{d}{dx} + a_2'(x)\right] - a_1'(x) - a_1(x)\frac{d}{dx} + a_0(x)\\ &= a_2'(x)\frac{d}{dx} + a_2(x)\frac{d^2}{dx^2} + a_2''(x) + a_2'(x)\frac{d}{dx} - a_1'(x) - a_1(x)\frac{d}{dx} + a_0(x)\\ &= a_2(x)\frac{d^2}{dx^2} + [2a_2'(x) - a_1(x)]\frac{d}{dx} + a_2''(x) - a_1'(x) + a_0(x).\end{aligned} \tag{10.17}$$

If

$$\mathscr{L}_x^\dagger = \mathscr{L}_x, \tag{10.18}$$

the operator $\mathscr{L}_x$ is called self-adjoint.

In order to prove that the Sturm-Liouville differential operator

$$\mathscr{S} = \frac{d}{dx}\left[p(x)\frac{d}{dx}\right] + q(x) = p(x)\frac{d^2}{dx^2} + p'(x)\frac{d}{dx} + q(x) \tag{10.19}$$

from Eq. (10.4) is self-adjoint, we verify Eq. (10.17) with $\mathscr{S}^\dagger$ taken from Eq. (10.16). Thereby, we identify $a_2(x) = p(x)$, $a_1(x) = p'(x)$, and $a_0(x) = q(x)$; hence

$$\begin{aligned}\mathscr{S}_x^\dagger &= a_2(x)\frac{d^2}{dx^2} + [2a_2'(x) - a_1(x)]\frac{d}{dx} + a_2''(x) - a_1'(x) + a_0(x)\\ &= p(x)\frac{d^2}{dx^2} + [2p'(x) - p'(x)]\frac{d}{dx} + p''(x) - p''(x) + q(x)\\ &= p(x)\frac{d^2}{dx^2} + p'(x)\frac{d}{dx}q(x)\\ &= \mathscr{S}_x.\end{aligned} \tag{10.20}$$

Alternatively we could argue from Eqs. (10.17) and (10.18), noting that a differential operator is self-adjoint if and only if

$$\begin{aligned}\mathscr{L}_x^\dagger &= a_2(x)\frac{d^2}{dx^2} - a_1(x)\frac{d}{dx} + a_0(x)\\ &= \mathscr{L}_x^\dagger = a_2(x)\frac{d^2}{dx^2} + [2a_2'(x) - a_1(x)]\frac{d}{dx} + a_2''(x) - a_1'(x) + a_0(x).\end{aligned} \tag{10.21}$$

By comparison of the coefficients,

$$\begin{aligned}a_2(x) &= a_2(x),\\ a_1(x) &= [2a_2'(x) - a_1(x)],\\ a_0(x) &= +a_2''(x) - a_1'(x) + a_0(x),\end{aligned} \tag{10.22}$$

and hence,

$$a_2'(x) = a_1(x), \tag{10.23}$$

which is exactly the form of the Sturm-Liouville differential operator.

10.4 *Sturm-Liouville transformation into Liouville normal form*

Let, for $x \in [a, b]$,

$$\begin{aligned}&[\mathscr{S}_x - \lambda\rho(x)]y(x) = 0,\\ &\frac{d}{dx}\left[p(x)\frac{d}{dx}\right]y(x) + [q(x) - \lambda\rho(x)]y(x) = 0,\\ &\left[p(x)\frac{d^2}{dx^2} + p'(x)\frac{d}{dx} + q(x) - \lambda\rho(x)\right]y(x) = 0,\\ &\left[\frac{d^2}{dx^2} + \frac{p'(x)}{p(x)}\frac{d}{dx} + \frac{q(x)-\lambda\rho(x)}{p(x)}\right]y(x) = 0\end{aligned} \tag{10.24}$$

be a second order differential equation of the Sturm-Liouville form [4].

This equation (10.24) can be written in the *Liouville normal form* containing no first order differentiation term

$$-\frac{d^2}{dt^2}w(t)+[\hat{q}(t)-\lambda]w(t)=0, \text{ with } t\in[0,c]. \tag{10.25}$$

It is obtained *via* the *Sturm-Liouville transformation*

$$\begin{aligned} \xi &= t(x)=\int_a^x\sqrt{\frac{\rho(s)}{p(s)}}ds,\\ w(t)&=\sqrt[4]{p(x(t))\rho(x(t))}\,y(x(t)), \end{aligned} \tag{10.26}$$

where

$$\hat{q}(t)=\frac{1}{\rho}\left[-q-\sqrt[4]{p\rho}\left(p\left(\frac{1}{\sqrt[4]{p\rho}}\right)'\right)'\right]. \tag{10.27}$$

The apostrophe represents derivation with respect to x.

Suppose we want to know the normalized eigenfunctions of

$$-x^2y''-3xy'-y=\lambda y, \text{ with } x\in[1,2] \tag{10.28}$$

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 $a_2(x)=-x^2$, $a_1(x)=-3x$, $a_0=-1$, $\rho=1$ and $f=\lambda y$; and hence

$$\begin{aligned} p(x)&=e^{\int\frac{(-3x)}{(-x^2)}dx}=e^{\int\frac{3}{x}dx}=e^{3\log x}=x^3,\\ q(x)&=p(x)\frac{(-1)}{(-x^2)}=x,\\ F(x)&=p(x)\frac{\lambda y}{(-x^2)}=-\lambda xy, \text{ and hence } \rho(x)=x. \end{aligned} \tag{10.29}$$

As a result we obtain the Sturm-Liouville form

$$\frac{1}{x}(-(x^3y')'-xy)=\lambda y. \tag{10.30}$$

In the next step we apply the Sturm-Liouville transformation

$$\begin{aligned} \xi&=t(x)=\int\sqrt{\frac{\rho(x)}{p(x)}}dx=\int\frac{dx}{x}=\log x,\\ w(t(x))&=\sqrt[4]{p(x(t))\rho(x(t))}\,y(x(t))=\sqrt[4]{x^4}\,y(x(t))=xy,\\ \hat{q}(t)&=\frac{1}{x}\left[-x-\sqrt[4]{x^4}\left(x^3\left(\frac{1}{\sqrt[4]{x^4}}\right)'\right)'\right]=0. \end{aligned} \tag{10.31}$$

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

$$-w''=\lambda w. \tag{10.32}$$

As an *Ansatz* for solving the Liouville normal form we use

$$w(\xi)=a\sin(\sqrt{\lambda}\xi)+b\cos(\sqrt{\lambda}\xi) \tag{10.33}$$

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 $\sqrt{\lambda_n}\log 2=n\pi$.

[4] 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

Thus the eigenvalues are

$$\lambda_n = \left(\frac{n\pi}{\log 2}\right)^2. \tag{10.34}$$

The associated eigenfunctions are

$$w_n(\xi) = a \sin\left[\frac{n\pi}{\log 2}\xi\right], \tag{10.35}$$

and thus

$$y_n = \frac{1}{x} a \sin\left[\frac{n\pi}{\log 2}\log x\right]. \tag{10.36}$$

We can check that they are orthonormal by inserting into Eq. (10.7) and verifying it; that is,

$$\int_1^2 \rho(x) y_n(x) y_m(x) dx = \delta_{nm}; \tag{10.37}$$

more explicitly,

$$\begin{aligned}
&\int_1^2 dx x \left(\frac{1}{x^2}\right) a^2 \sin\left(n\pi \frac{\log x}{\log 2}\right) \sin\left(m\pi \frac{\log x}{\log 2}\right) \\
&\quad [\text{variable substitution } u = \frac{\log x}{\log 2} \\
&\quad \frac{du}{dx} = \frac{1}{\log 2}\frac{1}{x},\; u = \frac{dx}{x \log 2}] \\
&\quad = \int_{u=0}^{u=1} du \log 2 a^2 \sin(n\pi u)\sin(m\pi u) \\
&\quad = \underbrace{a^2 \left(\frac{\log 2}{2}\right)}_{=1} \underbrace{2\int_0^1 du \sin(n\pi u)\sin(m\pi u)}_{=\delta_{nm}} \\
&\quad = \delta_{nm}.
\end{aligned} \tag{10.38}$$

Finally, with $a = \sqrt{\frac{2}{\log 2}}$ we obtain the solution

$$y_n = \sqrt{\frac{2}{\log 2}}\frac{1}{x}\sin\left(n\pi \frac{\log x}{\log 2}\right). \tag{10.39}$$

10.5 Varieties of Sturm-Liouville differential equations

A catalogue of Sturm-Liouville differential equations comprises the following *species*, among many others [5]. Some of these cases are tabellated as functions p, q, λ and ρ appearing in the general form of the Sturm-Liouville eigenvalue problem (10.6)

$$\begin{aligned}
&\mathcal{S}_x \phi(x) = -\lambda\rho(x)\phi(x), \text{ or} \\
&\frac{d}{dx}\left[p(x)\frac{d}{dx}\right]\phi(x) + [q(x) + \lambda\rho(x)]\phi(x) = 0
\end{aligned} \tag{10.40}$$

in Table 10.1.

[5] 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 *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	μ	$x^{\alpha}(1-x)^{\beta}$
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	α	e^{-x}
Associated Laguerre	$x^{k+1}e^{-x}$	0	$\alpha-k$	$x^k e^{-x}$
Hermite	xe^{-x^2}	0	2α	e^{-x}
Fourier (harmonic oscillator)	1	0	k^2	1
Schrödinger (hydrogen atom)	1	$l(l+1)x^{-2}$	μ	1

Table 10.1: Some varieties of differential equations expressible as Sturm-Liouville differential equations

11
Separation of variables

This chapter deals with the ancient alchemic suspicion of *"solve et coagula"* that it is possible to solve a problem by separation and joining together – for a counterexample see the Kochen-Specker theorem on page 69) – translated into the context of *partial differential equations;* that is, equations with derivatives of more than one variable. Already Descartes mentioned this sort of method in his *Discours de la méthode pour bien conduire sa raison et chercher la verité dans les sciences* (English translation: *Discourse on the Method of Rightly Conducting One's Reason and of Seeking Truth*) [1] stating that (in a newer translation [2])

> *[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.*

[1] Rene Descartes. *Discours de la méthode pour bien conduire sa raison et chercher la verité 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

[2] Rene Descartes. *The Philosophical Writings of Descartes. Volume 1*. Cambridge University Press, Cambridge, 1985. translated by John Cottingham, Robert Stoothoff and Dugald Murdoch

The method of separation of variables is one among a couple of strategies to solve differential equations [3], but it is a very important one in physics.

[3] 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. Funktionentheorie, Differentialgleichungen, Spezielle Funktionen*. Springer, Berlin, Heidelberg, fourth edition, 2001. URL http://www.springer.com/mathematics/analysis/book/978-3-540-41985-3

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

$$\begin{aligned} \mathscr{L}_{x,y}\psi(x,y) &= (\mathscr{L}_x+\mathscr{L}_y)\psi(x,y)=0, \text{ or} \\ \mathscr{L}_x\psi(x,y) &= -\mathscr{L}_y)\psi(x,y). \end{aligned} \tag{11.1}$$

Because in this case we may make a *multiplicative Ansatz*

$$\psi(x,y)=v(x)u(y). \tag{11.2}$$

Inserting (11.2) into (11.1) effectively separates the variable dependencies

$$\begin{aligned} &\mathscr{L}_x v(x)u(y) = -\mathscr{L}_y v(x)u(y),\\ &u(y)\left[\mathscr{L}_x v(x)\right] = -v(x)\left[\mathscr{L}_y u(y)\right],\\ &\tfrac{1}{v(x)}\mathscr{L}_x v(x) = -\tfrac{1}{u(y)}\mathscr{L}_y u(y) = a, \end{aligned} \tag{11.3}$$

with constant a, because $\frac{\mathscr{L}_x v(x)}{v(x)}$ does not depend on x, and $\frac{\mathscr{L}_y u(y)}{u(y)}$ 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,

$$\begin{aligned} &\tfrac{1}{v(x)}\mathscr{L}_x v(x) = a,\\ &\tfrac{1}{u(y)}\mathscr{L}_y u(y) = -a, \end{aligned} \tag{11.4}$$

or As a result, we can treat and integrate both sides separately; that is,

$$\begin{aligned} &\mathscr{L}_x v(x) - a v(x) = 0,\\ &\mathscr{L}_y u(y) + a u(y) = 0. \end{aligned} \tag{11.5}$$

This separation of variable *Ansatz* can be very often used whenever the *Laplace operator* $\Delta = \nabla\cdot\nabla$ is involved, since there the partial derivatives with respect to different variables occur in different summands.

For the sake of demonstration, let us consider a few examples.

1. Let us separate the homogenuous Laplace differential equation

$$\Delta\Phi = \frac{1}{u^2+v^2}\left(\frac{\partial^2\Phi}{\partial u^2}+\frac{\partial^2\Phi}{\partial v^2}\right)+\frac{\partial^2\Phi}{\partial z^2} = 0 \tag{11.6}$$

in parabolic cylinder coordinates (u,v,z) with $\mathbf{x} = \left(\frac{1}{2}(u^2-v^2), uv, z\right)$.

The separation of variables *Ansatz* is

$$\Phi(u,v,z) = \Phi_1(u)\Phi_2(v)\Phi_3(z).$$

Then,

$$\begin{aligned} \frac{1}{u^2+v^2}\left(\Phi_2\Phi_3\frac{\partial^2\Phi_1}{\partial u^2}+\Phi_1\Phi_3\frac{\partial^2\Phi_2}{\partial v^2}\right)+\Phi_1\Phi_2\frac{\partial^2\Phi}{\partial z^2} = 0\\ \frac{1}{u^2+v^2}\left(\frac{\Phi_1''}{\Phi_1}+\frac{\Phi_2''}{\Phi_2}\right) = -\frac{\Phi_3''}{\Phi_3} = \lambda = \text{const.} \end{aligned}$$

λ 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,

$$\frac{\Phi_1''}{\Phi_1} - \lambda u^2 = -\frac{\Phi_2''}{\Phi_2} + \lambda v^2 = l^2 = \text{const.}$$

with constant l for analoguous 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 homogenuous (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,

$$\begin{array}{l}
\frac{1}{a^2(\sinh^2 u+\sin^2 v)}\left(\Phi_2\Phi_3\frac{\partial^2\Phi_1}{\partial u^2} + \Phi_1\Phi_3\frac{\partial^2\Phi_2}{\partial v^2}\right) = -\Phi_1\Phi_2\frac{\partial^2\Phi}{\partial z^2},\\
\frac{1}{a^2(\sinh^2 u+\sin^2 v)}\left(\frac{\Phi_1''}{\Phi_1} + \frac{\Phi_2''}{\Phi_2}\right) = -\frac{\Phi_3''}{\Phi_3} = k^2 = \text{const.} \Longrightarrow \Phi_3'' + k^2\Phi_3 = 0\\
\frac{\Phi_1''}{\Phi_1} + \frac{\Phi_2''}{\Phi_2} = k^2a^2(\sinh^2 u + \sin^2 v),\\
\frac{\Phi_1''}{\Phi_1} - k^2a^2\sinh^2 u = -\frac{\Phi_2''}{\Phi_2} + k^2a^2\sin^2 v = l^2,
\end{array} \tag{11.7}$$

and finally,

$$\begin{array}{rcl}
\Phi_1'' & - & (k^2a^2\sinh^2 u + l^2)\Phi_1 = 0,\\
\Phi_2'' & - & (k^2a^2\sin^2 v - l^2)\Phi_2 = 0.
\end{array}$$

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 $\Phi(u, v, z, t) = \Phi_1(u)\Phi_2(v)\Phi_3(z)T(t)$

$$\begin{array}{l}
\Longrightarrow \frac{1}{a^2(\sinh^2 u+\sin^2 v)}\left(\frac{\Phi_1''}{\Phi_1} + \frac{\Phi_2''}{\Phi_2}\right) + \frac{\Phi_3''}{\Phi_3} = \frac{1}{c^2}\frac{T''}{T} = -\omega^2 = \text{const.},\\
\frac{1}{c^2}\frac{T''}{T} = -\omega^2 \Longrightarrow T'' + c^2\omega^2 T = 0,\\
\frac{1}{a^2(\sinh^2 u+\sin^2 v)}\left(\frac{\Phi_1''}{\Phi_1} + \frac{\Phi_2''}{\Phi_2}\right) = -\frac{\Phi_3''}{\Phi_3} - \omega^2 = k^2,\\
\Phi_3'' + (\omega^2 + k^2)\Phi_3 = 0\\
\frac{\Phi_1''}{\Phi_1} + \frac{\Phi_2''}{\Phi_2} = k^2a^2(\sinh^2 u + \sin^2 v)\\
\frac{\Phi_1''}{\Phi_1} - a^2k^2\sinh^2 u = -\frac{\Phi_2''}{\Phi_2} + a^2k^2\sin^2 v = l^2,
\end{array} \tag{11.8}$$

and finally,

$$\begin{array}{rcl}
\Phi_1'' & - & (k^2a^2\sinh^2 u + l^2)\Phi_1 = 0,\\
\Phi_2'' & - & (k^2a^2\sin^2 v - l^2)\Phi_2 = 0.
\end{array}$$

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

$$\begin{array}{l}
\frac{1}{a^2(\sinh^2 u+\sin^2 v)}\left(\frac{\Phi_1''}{\Phi_1} + \frac{\Phi_2''}{\Phi_2}\right) + \frac{\Phi_3''}{\Phi_3} = \frac{1}{D}\frac{T'}{T} = -\alpha^2 = \text{const.}\\
T = Ae^{-\alpha^2 Dt}\\
\Phi_3'' + (\alpha^2 + k^2)\Phi_3 = 0 \Longrightarrow \Phi_3'' = -(\alpha^2 + k^2)\Phi_3 \Longrightarrow \Phi_3 = Be^{i\sqrt{\alpha^2+k^2}\,z}
\end{array} \tag{11.9}$$

and finally,

$$
\begin{aligned}
\Phi_1'' &- (\alpha^2 k^2 \sinh^2 u + l^2)\Phi_1 &= 0 \\
\Phi_2'' &- (\alpha^2 k^2 \sin^2 v - l^2)\Phi_2 &= 0
\end{aligned}
$$

12
Special functions of mathematical physics

This chapter follows several good approaches [1]. For reference, consider [2].

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 parameter. 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 exhibis a high degree of "plasticity," as many elementary analytic functions can be expressed by them.

First, as a prerequisite, let us define the gamme function. Then we proceed to second order Fuchsian differential equations; followed by a rewriting of this Fuchsian differential equations into 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.

12.1 Gamma function

Although the gamma function $\Gamma(x)$ is an extension of the factorial function $n!$ as

$$\Gamma(n+1) = n! \text{ for } n \in \mathbb{N}, \tag{12.1}$$

[1] 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; 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; 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

[2] 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 & Hall Press, Boca Raton, London, New York, 2008; and I. S. Gradshteyn and I. M. Ryzhik. *Tables of Integrals, Series, and Products, 6th ed.* Academic Press, San Diego, CA, 2000

it is also for real or complex arguments.

Let us first define the *shifted factorial* or, by another naming, the *Pochhammer symbol*

$$(a)_0 = 1, \quad (a)_n = a(a+1)\cdots(a+n-1), \text{ for } n > 0, \tag{12.2}$$

where a can be any real or complex number.

With this definition,

$$\begin{aligned} z!(z+1)_n &= 1\cdot 2\cdots z\cdot(z+1)((z+1)+1)\cdots((z+1)+n-1)\\ &= 1\cdot 2\cdots z\cdot(z+1)(z+2)\cdots(z+n)\\ &= (z+n)!, \text{ or}\\ z! &= \tfrac{(z+n)!}{(z+1)_n}. \end{aligned} \tag{12.3}$$

Since

$$\begin{aligned} (z+n)! &= (n+z)!\\ &= 1\cdot 2\cdots n\cdot(n+1)(n+2)\cdots(n+z)\\ &= n!\cdot(n+1)(n+2)\cdots(n+z)\\ &= n!\cdot(n+1)(n+2)\cdots(n+z)\\ &= n!(n+1)_z, \end{aligned} \tag{12.4}$$

we can rewrite Eq. (12.3) into

$$z! = \frac{n!(n+1)_z}{(z+1)_n} = \frac{n!n^z}{(z+1)_n}\frac{(n+1)_z}{n^z}. \tag{12.5}$$

Since the latter factor, for large n, converges as ["$O(x)$" means "of the order of x"]

$$\begin{aligned} \tfrac{(n+1)_z}{n^z} &= \tfrac{(n+1)((n+1)+1)\cdots((n+1)+z-1)}{n^z}\\ &= \tfrac{n^z+O(n^{z-1})}{n^z}\\ &= \tfrac{n^z}{n^z}+\tfrac{O(n^{z-1})}{n^z}\\ &= 1+O(n^{-1}) \stackrel{n\to\infty}{\longrightarrow} 1, \end{aligned} \tag{12.6}$$

in this limit, Eq. (12.5) can be written as

$$z! = \lim_{n\to\infty} z! = \lim_{n\to\infty}\frac{n!n^z}{(z+1)_n}. \tag{12.7}$$

Hence, for all $z \in \mathbb{C}$ which are not equal to a negative integer – that is, $z \neq 0, -1, -2, \ldots$ – we can, in analogy to the "classical factorial," define a "factorial function shifted by one" as

$$\begin{aligned} \Gamma(z+1) &= \lim_{n\to\infty}\tfrac{n!n^z}{(z+1)_n}, \text{ or}\\ \Gamma(z) &= \lim_{n\to\infty}\tfrac{n!n^{z-1}}{(z)_n}. \end{aligned} \tag{12.8}$$

Hence we effectively express $z!$ in Eq. (12.3) in terms of $\Gamma(z+1)$, which also implies that

$$\Gamma(z+1) = z\Gamma(z), \tag{12.9}$$

as well as $\Gamma(n+1) = n!$ for $n \in \mathbb{N}$. Note that, since

$$(1)_n = 1(1+1)(1+2)\cdots(1-n-1) = n!, \tag{12.10}$$

Eq. (12.8) yields

$$\Gamma(1) = \lim_{n\to\infty} \frac{n!n^0}{(1)_n} = \lim_{n\to\infty} \frac{n!}{n!} = 1. \tag{12.11}$$

We state without proof that, for positive real parts $\Re x$, $\Gamma(x)$ has an integral representation as

$$\Gamma(x) = \int_0^\infty t^{x-1} e^{-t} dt. \tag{12.12}$$

Also the next formulae

$$\begin{aligned}
&\Gamma(\tfrac{1}{2}) = \sqrt{\pi}, \text{ or, more generally,}\\
&\Gamma(\tfrac{n}{2}) = \sqrt{\pi}\tfrac{(n-2)!!}{2^{(n-1)/2}}, \text{ for } n>0, \text{ and}\\
&\Gamma(x)\Gamma(1-x) = \tfrac{\pi}{\sin(\pi x)}, \text{ Euler's reflection formula,}
\end{aligned} \tag{12.13}$$

are stated without proof.

Here, the *double factorial* is defined by

$$n!! = \begin{cases}
1 \text{ for } n=-1,0, \text{ and}\\
2\cdot 4\cdots(n-2)\cdot n\\
\qquad = (2k)!! = \prod_{i=1}^{k}(2i)\\
\qquad = 2^{n/2}\left(1\cdot 2\cdots \frac{(n-2)}{2}\cdot\frac{n}{2}\right)\\
\qquad = k!2^k \text{ for positive even } n=2k, k\geq 1, \text{ and}\\
1\cdot 3\cdots(n-2)\cdot n\\
\qquad = (2k-1)!! = \prod_{i=1}^{k}(2i-1)\\
\qquad = \frac{1\cdot 2\cdots(2k-2)\cdot(2k-1)\cdot(2k)}{(2k)!!}\\
\qquad = \frac{(2k)!}{k!2^k} \text{ for odd positive } n=2k-1, k\geq 1.
\end{cases} \tag{12.14}$$

Stirling's formula [again, $O(x)$ means "of the order of x"]

$$\begin{aligned}
&\log n! = n\log n - n + O(\log(n)), \text{ or}\\
&n! \stackrel{n\to\infty}{\longrightarrow} \sqrt{2\pi n}\left(\tfrac{n}{e}\right)^n, \text{ or, more generally,}\\
&\log\Gamma(x) = \sqrt{\tfrac{2\pi}{x}}\left(\tfrac{x}{e}\right)^x\left(1+O\left(\tfrac{1}{x}\right)\right)
\end{aligned} \tag{12.15}$$

is stated without proof.

12.2 Beta function

The *beta function,* also called the *Euler integral of the first kind,* is a special function defined by

$$B(x,y) = \int_0^1 t^{x-1}(1-t)^{y-1} dt = \frac{\Gamma(x)\Gamma(y)}{\Gamma(x+y)} \text{ for } \Re x, \Re y > 0 \tag{12.16}$$

No proof of the identity of the two representations in terms of an integral, and of Γ-functions is given.

12.3 Fuchsian differential equations

Many differential equations of theoretical physics are Fuchsian equations. We shall therefore study this class in some generality.

12.3.1 *Regular, regular singular, and irregular singular point*

Consider the homogenuous differential equation [Eq. (10.1) on page 155 is inhomogenuos]

$$\mathscr{L}_x y(x) = a_2(x)\frac{d^2}{dx^2}y(x) + a_1(x)\frac{d}{dx}y(x) + a_0(x)y(x) = 0. \tag{12.17}$$

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 (12.17) by $a_2(x)$ and rewite it

$$\frac{1}{a_2(x)}\mathscr{L}_x y(x) = \frac{d^2}{dx^2}y(x) + d(x)\frac{d}{dx}y(x) + e(x)y(x) = 0, \tag{12.18}$$

with $d(x) = a_1(x)/a_2(x)$ and $e(x) = a_0(x)/a_2(x)$.

If, however, $a_2(x_0) = 0$ and $a_1(x_0)$ or $a_0(x_0)$ are nonzero, the x_0 is called *singular point* of (12.17). The simplest case is if $a_0(x_0)$ has a *simple zero* at x_0; then both $d(x)$ and $e(x)$ in (12.18) 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. (12.17) if

$$\lim_{x\to x_0}\frac{(x-x_0)a_1(x)}{a_2(x)}, \text{ as well as } \lim_{x\to x_0}\frac{(x-x_0)^2 a_0(x)}{a_2(x)} \tag{12.19}$$

both exist. If any one of these limits does not exist, the singular point is an *irregular singular point*.

A very important case is the case of the *Fuchsian differential equation*, where in (12.18)

- $d(x)$ has at most a *single pole*, and
- $e(x)$ has at most a *double pole*.

The simples realization of this case is for

$$a_2(x) = a(x-x_0),$$
$$a_1(x) = b(x-x_0),$$
$$a_0(x) = c.$$

Stated differently, a linear ordinary differential equation is called Fuchsian if every singular point, including infinity, is regular. Hence, in Eq. (12.18), the equation is of the Fuchsian class if the coefficients are of the form

$$\begin{aligned} d(x) &= \textstyle\prod_{j=1}^k \frac{q_1(x)}{(x-x_j)}, \text{ and} \\ e(x) &= \textstyle\prod_{j=1}^k \frac{q_0(x)}{(x-x_j)^2}, \end{aligned} \tag{12.20}$$

where the $x_1,\ldots,x_k$ are k (singular) points, and $q_1(x)$ and $q_0(x)$ are polynomials of degree less then or equal to k and $2k$, respectively. Hence, the coefficients of Fuchsian equations must be rational functions; that is, they must be of the form $\frac{P(x)}{Q(x)}$, where $P(x)$ and $Q(x)$ are polynomials in x with real coefficients.

The *hypergeometric differential equation* is a *Fuchsian differential equation* which has at most *three regular singularities*, including infinity, at 0, 1, and ∞ [3].

[3] 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

12.3.2 *Power series solution*

Now let us get more concrete about the solution of Fuchsian equations by *power series*.

In order to get a feeling for power series solutions of differential equations, consider the "first order" Fuchsian equation [4]

$$y' - \lambda y = 0. \tag{12.21}$$

[4] Ron Larson and Bruce H. Edwards. *Calculus*. Brooks/Cole Cengage Learning, Belmont, CA, 9th edition, 2010. ISBN 978-0-547-16702-2

Make the *Ansatz* that the solution can be expanded into a power series of the form

$$y(x) = \sum_{j=0}^{\infty} a_j x^j. \tag{12.22}$$

Then, Eq. (12.21) can be written as

$$\begin{aligned}
&\left(\frac{d}{dx}\sum_{j=0}^{\infty} a_j x^j\right) - \lambda \sum_{j=0}^{\infty} a_j x^j = 0,\\
&\sum_{j=0}^{\infty} j a_j x^{j-1} - \lambda \sum_{j=0}^{\infty} a_j x^j = 0,\\
&\sum_{j=1}^{\infty} j a_j x^{j-1} - \lambda \sum_{j=0}^{\infty} a_j x^j = 0,\\
&\sum_{m=j-1=0}^{\infty} (m+1) a_{m+1} x^m - \lambda \sum_{j=0}^{\infty} a_j x^j = 0,\\
&\sum_{j=0}^{\infty} (j+1) a_{j+1} x^j - \lambda \sum_{j=0}^{\infty} a_j x^j = 0,
\end{aligned} \tag{12.23}$$

and hence, by comparing the coefficients of x^j, for $n \geq 0$,

$$\begin{aligned}
&(j+1) a_{j+1} = \lambda a_j, \text{ or}\\
&a_{j+1} = \frac{\lambda a_j}{j+1} = a_0 \frac{\lambda^{j+1}}{(j+1)!}, \text{ and}\\
&a_j = a_0 \frac{\lambda^j}{j!}.
\end{aligned} \tag{12.24}$$

Therefore,

$$y(x) = \sum_{j=0}^{\infty} a_0 \frac{\lambda^j}{j!} x^j = a_0 \sum_{j=0}^{\infty} \frac{(\lambda x)^j}{j!} = a_0 e^{\lambda x}. \tag{12.25}$$

In the Fuchsian case let us consider the following *generalized power series Ansatz* around a regular singular point x_0, which can be motivated by Eq. (12.20), and by the *Laurent series expansion* (6.23)–(6.25) on page 117:

$$\begin{aligned}
&d(x) = \frac{A_1(x)}{x-x_0} = \sum_{j=0}^{\infty} \alpha_j (x-x_0)^{j-1}, \text{ for } 0 < |x-x_0| < r_1,\\
&e(x) = \frac{A_2(x)}{(x-x_0)^2} = \sum_{j=0}^{\infty} \beta_j (x-x_0)^{j-2}, \text{ for } 0 < |x-x_0| < r_2,\\
&y(x) = (x-x_0)^{\sigma} \sum_{l=0}^{\infty} w_l (x-x_0)^l = \sum_{l=0}^{\infty} w_l (x-x_0)^{l+\sigma}, \text{ with } w_0 \neq 0.
\end{aligned} \tag{12.26}$$

Eq. (12.18) then becomes

$$
\begin{aligned}
&\frac{d^2}{dx^2}y(x)+d(x)\frac{d}{dx}y(x)+e(x)y(x)=0,\\
&\left[\frac{d^2}{dx^2}+\sum_{j=0}^{\infty}\alpha_j(x-x_0)^{j-1}\frac{d}{dx}y(x)+\sum_{j=0}^{\infty}\beta_j(x-x_0)^{j-2}\right]\sum_{l=0}^{\infty}w_l(x-x_0)^{l+\sigma}=0,\\
&(l+\sigma)(l+\sigma-1)\sum_{l=0}^{\infty}w_l(x-x_0)^{l+\sigma-2}\\
&\qquad+\left[(l+\sigma)\sum_{l=0}^{\infty}w_l(x-x_0)^{l+\sigma-1}\right]\sum_{j=0}^{\infty}\alpha_j(x-x_0)^{j-1}\\
&\qquad+\left[\sum_{l=0}^{\infty}w_l(x-x_0)^{l+\sigma}\right]\sum_{j=0}^{\infty}\beta_j(x-x_0)^{j-2}=0,\\
&(l+\sigma)(l+\sigma-1)\sum_{l=0}^{\infty}w_l(x-x_0)^{l+\sigma-2}\\
&\qquad+\left[(l+\sigma)\sum_{l=0}^{\infty}w_l(x-x_0)^{l+\sigma-1}\right]\sum_{j=0}^{\infty}\alpha_j(x-x_0)^{j-1}\\
&\qquad+\left[\sum_{l=0}^{\infty}w_l(x-x_0)^{l+\sigma}\right]\sum_{j=0}^{\infty}\beta_j(x-x_0)^{j-2}=0,\\
&(x-x_0)^{\sigma-2}\sum_{l=0}^{\infty}(x-x_0)^l\,[(l+\sigma)(l+\sigma-1)w_l\\
&\qquad+(l+\sigma)w_l\sum_{j=0}^{\infty}\alpha_j(x-x_0)^j\\
&\qquad+w_l\sum_{j=0}^{\infty}\beta_j(x-x_0)^j\Big]=0,\\
&(x-x_0)^{\sigma-2}\sum_{l=0}^{\infty}(l+\sigma)(l+\sigma-1)w_l(x-x_0)^l\\
&\qquad+\sum_{l=0}^{\infty}(l+\sigma)w_l\sum_{j=0}^{\infty}\alpha_j(x-x_0)^{l+j}\\
&\qquad+\sum_{l=0}^{\infty}w_l\sum_{j=0}^{\infty}\beta_j(x-x_0)^{l+j}=0.
\end{aligned}
$$

Next, in order to reach a common power of $(x-x_0)$, we perform an index identification $l=m$ in the first summand, as well as an index shift

$$l+j=m,\; j=m-l,\text{ since } l\ge 0 \text{ and } j\ge 0 \Rightarrow 0\le l\le m$$

in the second and third summands (where the order of the sums change):

$$
\begin{aligned}
&(x-x_0)^{\sigma-2}\sum_{l=0}^{\infty}(l+\sigma)(l+\sigma-1)w_l(x-x_0)^l\\
&\qquad+\sum_{j=0}^{\infty}\sum_{l=0}^{\infty}(l+\sigma)w_l\alpha_j(x-x_0)^{l+j}\\
&\qquad+\sum_{j=0}^{\infty}\sum_{l=0}^{\infty}w_l\beta_j(x-x_0)^{l+j}=0,\\
&(x-x_0)^{\sigma-2}\sum_{m=0}^{\infty}(m+\sigma)(m+\sigma-1)w_m(x-x_0)^m\\
&\qquad+\sum_{m=0}^{\infty}\sum_{l=0}^{m}(l+\sigma)w_l\alpha_{m-l}(x-x_0)^{l+m-l}\\
&\qquad+\sum_{m=0}^{\infty}\sum_{l=0}^{m}w_l\beta_{m-l}(x-x_0)^{l+m-l}=0,\\
&(x-x_0)^{\sigma-2}\left\{\sum_{m=0}^{\infty}(x-x_0)^m\,[(m+\sigma)(m+\sigma-1)w_m\right.\\
&\qquad+\sum_{l=0}^{m}(l+\sigma)w_l\alpha_{m-l}\\
&\qquad\left.+\sum_{l=0}^{m}w_l\beta_{m-l}\Big]\right\}=0,\\
&(x-x_0)^{\sigma-2}\left\{\sum_{m=0}^{\infty}(x-x_0)^m\,[(m+\sigma)(m+\sigma-1)w_m\right.\\
&\qquad\left.+\;\sum_{l=0}^{m}w_l\big((l+\sigma)\alpha_{m-l}+\beta_{m-l}\big)\Big]\right\}=0.
\end{aligned}
\tag{12.27}
$$

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 $[\cdots]$–brackets in Eq. (12.27) vanish *individually.* In particular, for $m=0$ and $w_0\neq 0$,

$$
\begin{aligned}
&(0+\sigma)(0+\sigma-1)w_0+w_0\big((0+\sigma)\alpha_0+\beta_0\big)=0\\
&\sigma(\sigma-1)+\sigma\alpha_0+\beta_0=f_0(\sigma)=0.
\end{aligned}
\tag{12.28}
$$

The *radius of convergence* of the sulution will, in accordance with the Laurent series expansion, extend to the next singularity.

Note that in Eq. (12.28) we have defined $f_0(\sigma)$ which we will use now. Furthermore, for successive m, and with the definition of $f_k(\sigma) = \alpha_k\sigma + \beta_k$, we obtain the sequence of linear equations

$$\begin{aligned}
&w_0 f_0(\sigma) = 0\\
&w_1 f_0(\sigma+1) + w_0 f_1(\sigma) = 0,\\
&w_2 f_0(\sigma+2) + w_1 f_1(\sigma+1) + w_0 f_2(\sigma) = 0,\\
&\vdots\\
&w_n f_0(\sigma+n) + w_{n-1} f_1(\sigma+n-1) + \cdots + w_0 f_n(\sigma) = 0.
\end{aligned} \tag{12.29}$$

which can be used for an inductive determination of the coefficients w_k.

Eq. (12.28) is a quadratic equation $\sigma^2 + \sigma(\alpha_0 - 1) + \beta_0 = 0$ for the *characteristic exponents*

$$\sigma_{1,2} = \frac{1}{2}\left[1 - \alpha_0 \pm \sqrt{(1-\alpha_0)^2 - 4\beta_0}\right] \tag{12.30}$$

We state without proof that, if the difference of the characteristic exponents

$$\sigma_1 - \sigma_2 = \sqrt{(1-\alpha_0)^2 - 4\beta_0} \tag{12.31}$$

is *nonzero* and *not* an integer, then the two solutions found from $\sigma_{1,2}$ through the generalized series Ansatz (12.26) are linear independent.

If, however $\sigma_1 = \sigma_2 + n$ with $n \in \mathbb{Z}$ then we can only obtain a *single* solution of the Fuchsian equation. In order to obtain anotherlinear independent solution we have to employ the d'Alambert reduction, which is a general method to obtain another, linear independent solution $y_2(x)$ from an existing particular solution $y_1(x)$ by

$$y_2(x) = y_1(x) \int_x u(s)ds. \tag{12.32}$$

Inserting $y_2(x)$ from (12.32) into the Fuchsian equation (12.18), and using the fact that by assumption $y_1(x)$ is a solution of it, yields

$$
\begin{aligned}
&\tfrac{d^2}{dx^2}y_2(x)+d(x)\tfrac{d}{dx}y_2(x)+e(x)y_2(x)=0,\\
&\tfrac{d^2}{dx^2}y_1(x)\int_x u(s)ds+d(x)\tfrac{d}{dx}y_1(x)\int_x u(s)ds+e(x)y_1(x)\int_x u(s)ds=0,\\
&\tfrac{d}{dx}\left\{\left[\tfrac{d}{dx}y_1(x)\right]\int_x u(s)ds+y_1(x)u(x)\right\}\\
&\qquad+d(x)\left[\tfrac{d}{dx}y_1(x)\right]\int_x u(s)ds+y_1(x)u(x)+e(x)y_1(x)\int_x u(s)ds=0,\\
&\left[\tfrac{d^2}{dx^2}y_1(x)\right]\int_x u(s)ds+\left[\tfrac{d}{dx}y_1(x)\right]u(x)+\left[\tfrac{d}{dx}y_1(x)\right]u(x)+y_1(x)\left[\tfrac{d}{dx}u(x)\right]\\
&\qquad+d(x)\left[\tfrac{d}{dx}y_1(x)\right]\int_x u(s)ds+d(x)y_1(x)u(x)+e(x)y_1(x)\int_x u(s)ds=0,\\
&\left[\tfrac{d^2}{dx^2}y_1(x)\right]\int_x u(s)ds+d(x)\left[\tfrac{d}{dx}y_1(x)\right]\int_x u(s)ds+e(x)y_1(x)\int_x u(s)ds\\
&\qquad+d(x)y_1(x)u(x)+\left[\tfrac{d}{dx}y_1(x)\right]u(x)+\left[\tfrac{d}{dx}y_1(x)\right]u(x)+y_1(x)\left[\tfrac{d}{dx}u(x)\right]=0,\\
&\left[\tfrac{d^2}{dx^2}y_1(x)\right]\int_x u(s)ds+d(x)\left[\tfrac{d}{dx}y_1(x)\right]\int_x u(s)ds+e(x)y_1(x)\int_x u(s)ds\\
&\qquad+y_1(x)\left[\tfrac{d}{dx}u(x)\right]+2\left[\tfrac{d}{dx}y_1(x)\right]u(x)+d(x)y_1(x)u(x)=0,\\
&\left\{\left[\tfrac{d^2}{dx^2}y_1(x)\right]+d(x)\left[\tfrac{d}{dx}y_1(x)\right]+e(x)y_1(x)\right\}\int_x u(s)ds\\
&\qquad+y_1(x)\left[\tfrac{d}{dx}u(x)\right]+\left\{2\left[\tfrac{d}{dx}y_1(x)\right]+d(x)y_1(x)\right\}u(x)=0,\\
&y_1(x)\left[\tfrac{d}{dx}u(x)\right]+\left\{2\left[\tfrac{d}{dx}y_1(x)\right]+d(x)y_1(x)\right\}u(x)=0,
\end{aligned}
\tag{12.33}
$$

and finally,

$$u'(x)+u(x)\left\{2\frac{y_1'(x)}{y_1(x)}+d(x)\right\}=0. \tag{12.34}$$

Let us consider some examples involving Fuchsian equations of the second order.

1. Let $w''+p_1(z)w'+p_2(z)w=0$ a Fuchsian equation. Derive from the Laurent series expansion of $p_1(z)$ and $p_2(z)$ with Cauchy's integral formula the following equations:

$$
\begin{aligned}
\alpha_0&=\lim_{z\to z_0}(z-z_0)p_1(z),\\
\beta_0&=\lim_{z\to z_0}(z-z_0)^2p_2(z),
\end{aligned}
\tag{12.35}
$$

   where z_0 is a regular singular point.

   Let us consider α_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 : $n=k+1$ ($\Longrightarrow k=n-1$) and $\alpha_n:=\tilde{a}_{n-1}$; 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

$$p_1(z) = \frac{a_1(z)}{(z-z_0)} = \frac{p_1(z)(z-z_0)}{(z-z_0)}$$

and

$$\alpha_0 = \frac{1}{2\pi i}\oint \frac{p_1(s)(s-z_0)}{(s-z_0)}ds,$$

where $p_1(s)(s-z_0)$ is analytic around z_0; hence we can apply Cauchy's integral formula:

$$\alpha_0 = \lim_{s\to z_0} p_1(s)(s-z_0)$$

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 $z \to z_0$,

$$\lim_{z\to z_0}(z-z_0)p_1(z) = \alpha_n$$

Let us consider β_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 : $n = k+2$ ($\Longrightarrow k = n-2$) and $\beta_n := \tilde{b}_{n-2}$. 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

$$p_2(z) = \frac{a_2(z)}{(z-z_0)^2} = \frac{p_2(z)(z-z_0)^2}{(z-z_0)^2}$$

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

$$\beta_0 = \lim_{s\to z_0} p_2(s)(s-z_0)^2.$$

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 $z \to z_0$, yields

$$\lim_{z\to z_0} (z-z_0)^2 p_2(z) = \beta_n$$

2. For $z = \infty$, transform the Fuchsian equation $w'' + p_1(z)w' + p_2(z)w = 0$ above into the new variable $t = \frac{1}{z}$.

$$
\begin{aligned}
t = \frac{1}{z},\; z = \frac{1}{t},\; u(t) := w\left(\frac{1}{t}\right) = w(z)\\
\frac{dz}{dt} = -\frac{1}{t^2} \Longrightarrow \frac{d}{dz} = -t^2\frac{d}{dt}\\
\frac{d^2}{dz^2} = -t^2\frac{d}{dt}\left(-t^2\frac{d}{dt}\right) = -t^2\left(-2t\frac{d}{dt} - t^2\frac{d^2}{dt^2}\right) = 2t^3\frac{d}{dt} + t^4\frac{d^2}{dt^2}\\
w'(z) = \frac{d}{dz}w(z) = -t^2\frac{d}{dt}u(t) = -t^2u'(t)\\
w''(z) = \frac{d^2}{dz^2}w(z) = \left(2t^3\frac{d}{dt} + t^4\frac{d^2}{dt^2}\right)u(t) = 2t^3u'(t) + t^4u''(t)
\end{aligned}
$$

Insertion into the Fuchsian equation $w'' + p_1(z)w' + p_2(z)w = 0$ yields

$$2t^3u' + t^4u'' + p_1\left(\frac{1}{t}\right)(-t^2u') + p_2\left(\frac{1}{t}\right)u = 0,$$

and hence,

$$u'' + \left[\frac{2}{t} - \frac{p_1\left(\frac{1}{t}\right)}{t^2}\right]u' + \frac{p_2\left(\frac{1}{t}\right)}{t^4}u = 0$$

with $\tilde{p}_1(t) := \left[\frac{2}{t} - \frac{p_1\left(\frac{1}{t}\right)}{t^2}\right]$ und $\tilde{p}_2(t) := \frac{p_2\left(\frac{1}{t}\right)}{t^4}$ ist $u'' + \tilde{p}_1(t)u' + \tilde{p}_2(t)u = 0$.

3. Find out whether the following differential equations are Fuchsian, and enumerate the regular singular points:

$$
\begin{aligned}
&zw'' + (1-z)w' = 0,\\
&z^2w'' + zw' - \nu^2 w = 0,\\
&z^2(1+z)^2w'' + 2z(z+1)(z+2)w' - 4w = 0,\\
&2z(z+2)w'' + w' - zw = 0.
\end{aligned}
\tag{12.36}
$$

ad 1: $zw'' + (1-z)w' = 0 \Longrightarrow w'' + \frac{(1-z)}{z}w' = 0$

$z = 0$:

$$\alpha_0 = \lim_{z\to 0} z\frac{(1-z)}{z} = 1, \quad \beta_0 = \lim_{z\to 0} z^2\cdot 0 = 0.$$

The equation for the characteristic exponent is

$$\sigma(\sigma-1) + \sigma\alpha_0 + \beta_0 = 0 \Longrightarrow \sigma^2 - \sigma + \sigma = 0 \Longrightarrow \sigma_{1,2} = 0.$$

$z = \infty$: $z = \frac{1}{t}$

$$\tilde{p}_1(t) = \frac{2}{t} - \frac{\frac{\left(1-\frac{1}{t}\right)}{\frac{1}{t}}}{t^2} = \frac{2}{t} - \frac{\left(1-\frac{1}{t}\right)}{t} = \frac{1}{t} + \frac{1}{t^2} = \frac{t+1}{t^2}$$

$\Longrightarrow$ not Fuchsian.

ad 2: $z^2 w'' + z w' - v^2 w = 0 \Longrightarrow w'' + \frac{1}{z} w' - \frac{v^2}{z^2} w = 0.$

$z = 0$:

$$\alpha_0 = \lim_{z\to 0} z \frac{1}{z} = 1, \quad \beta_0 = \lim_{z\to 0} z^2 \left(-\frac{v^2}{z^2}\right) = -v^2.$$

$$\Longrightarrow \sigma^2 - \sigma + \sigma - v^2 = 0 \Longrightarrow \sigma_{1,2} = \pm v$$

$z = \infty$: $z = \frac{1}{t}$

$$\begin{aligned} \tilde{p}_1(t) &= \frac{2}{t} - \frac{1}{t^2} t = \frac{1}{t} \\ \tilde{p}_2(t) &= \frac{1}{t^4}\left(-t^2 v^2\right) = -\frac{v^2}{t^2} \end{aligned}$$

$$\Longrightarrow u'' + \frac{1}{t} u' - \frac{v^2}{t^2} u = 0 \Longrightarrow \sigma_{1,2} = \pm v$$

$\Longrightarrow$ Fuchsian equation.

ad 3:

$$z^2(1+z)^2 w'' + 2z(z+1)(z+2) w' - 4w = 0 \Longrightarrow w'' + \frac{2(z+2)}{z(z+1)} w' - \frac{4}{z^2(1+z)^2} w = 0$$

$z = 0$:

$$\alpha_0 = \lim_{z\to 0} z \frac{2(z+2)}{z(z+1)} = 4, \quad \beta_0 = \lim_{z\to 0} z^2 \left(-\frac{4}{z^2(1+z)^2}\right) = -4.$$

$$\Longrightarrow \sigma(\sigma-1) + 4\sigma - 4 = \sigma^2 + 3\sigma - 4 = 0 \Longrightarrow \sigma_{1,2} = \frac{-3 \pm \sqrt{9+16}}{2} = \begin{cases} -4 \\ +1 \end{cases}$$

$z = -1$:

$$\alpha_0 = \lim_{z\to -1} (z+1) \frac{2(z+2)}{z(z+1)} = -2, \quad \beta_0 = \lim_{z\to -1} (z+1)^2 \left(-\frac{4}{z^2(1+z)^2}\right) = -4.$$

$$\Longrightarrow \sigma(\sigma-1) - 2\sigma - 4 = \sigma^2 - 3\sigma - 4 = 0 \Longrightarrow \sigma_{1,2} = \frac{3 \pm \sqrt{9+16}}{2} = \begin{cases} +4 \\ -1 \end{cases}$$

$z = \infty$:

$$\begin{aligned} \tilde{p}_1(t) &= \frac{2}{t} - \frac{1}{t^2} \frac{2\left(\frac{1}{t}+2\right)}{\frac{1}{t}\left(\frac{1}{t}+1\right)} = \frac{2}{t} - \frac{2\left(\frac{1}{t}+2\right)}{1+t} = \frac{2}{t}\left(1 - \frac{1+2t}{1+t}\right) \\ \tilde{p}_2(t) &= \frac{1}{t^4}\left(-\frac{4}{\frac{1}{t^2}\left(1+\frac{1}{t}\right)^2}\right) = -\frac{4}{t^2} \frac{t^2}{(t+1)^2} = -\frac{4}{(t+1)^2} \end{aligned}$$

$$\Longrightarrow u'' + \frac{2}{t}\left(1 - \frac{1+2t}{1+t}\right)u' - \frac{4}{(t+1)^2}u = 0$$

$$\alpha_0 = \lim_{t\to 0} t\frac{2}{t}\left(1-\frac{1+2t}{1+t}\right) = 0, \quad \beta_0 = \lim_{t\to 0} t^2\left(-\frac{4}{(t+1)^2}\right) = 0.$$

$$\Longrightarrow \sigma(\sigma-1) = 0 \Longrightarrow \sigma_{1,2} = \begin{cases} 0 \\ 1 \end{cases}$$

$\Longrightarrow$ Fuchsian equation.

ad 4:

$$2z(z+2)w'' + w' - zw = 0 \Longrightarrow w'' + \frac{1}{2z(z+2)}w' - \frac{1}{2(z+2)}w = 0$$

$z = 0$:

$$\alpha_0 = \lim_{z\to 0} z\frac{1}{2z(z+2)} = \frac{1}{4}, \quad \beta_0 = \lim_{z\to 0} z^2\frac{-1}{2(z+2)} = 0.$$

$$\Longrightarrow \sigma^2 - \sigma + \frac{1}{4}\sigma = 0 \Longrightarrow \sigma^2 - \frac{3}{4}\sigma = 0 \Longrightarrow \sigma_1 = 0, \sigma_2 = \frac{3}{4}.$$

$z = -2$:

$$\alpha_0 = \lim_{z\to -2}(z+2)\frac{1}{2z(z+2)} = -\frac{1}{4}, \quad \beta_0 = \lim_{z\to -2}(z+2)^2\frac{-1}{2(z+2)} = 0.$$

$$\Longrightarrow \sigma_1 = 0, \quad \sigma_2 = \frac{5}{4}.$$

$z = \infty$:

$$\begin{aligned} \tilde{p}_1(t) &= \frac{2}{t} - \frac{1}{t^2}\left(\frac{1}{2\frac{1}{t}\left(\frac{1}{t}+2\right)}\right) = \frac{2}{t} - \frac{1}{2(1+2t)} \\ \tilde{p}_2(t) &= \frac{1}{t^4}\frac{(-1)}{2\left(\frac{1}{t}+2\right)} = -\frac{1}{2t^3(1+2t)} \end{aligned}$$

$\Longrightarrow$ no Fuchsian. Klasse!

4. Determine the solutions of

$$z^2w'' + (3z+1)w' + w = 0$$

around the regular singular points.

The singularities are at $z = 0$ and $z = \infty$.

Singularities at $z = 0$:

$$p_1(z) = \frac{3z+1}{z^2} = \frac{a_1(z)}{z} \qquad \text{mit} \qquad a_1(z) = 3 + \frac{1}{z}$$

$p_1(z)$ 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 $z = \frac{1}{t}$, $w(z) \to u(t)$:

$$u''(t) + \left[\frac{2}{t} - \frac{1}{t^2} p_1\left(\frac{1}{t}\right)\right] \cdot u'(t) + \frac{1}{t^4} p_2\left(\frac{1}{t}\right) \cdot u(t) = 0.$$

The new coefficient functions are

$$\begin{aligned}\tilde{p}_1(t) &= \frac{2}{t} - \frac{1}{t^2} p_1\left(\frac{1}{t}\right) = \frac{2}{t} - \frac{1}{t^2}(3t + t^2) = \frac{2}{t} - \frac{3}{t} - 1 = -\frac{1}{t} - 1 \\ \tilde{p}_2(t) &= \frac{1}{t^4} p_2\left(\frac{1}{t}\right) = \frac{t^2}{t^4} = \frac{1}{t^2}\end{aligned}$$

- check whether this is a regular singular point:

$$\begin{array}{lll}\tilde{p}_1(t) = -\frac{1+t}{t} = \frac{\tilde{a}_1(t)}{t} & \text{mit } \tilde{a}_1(t) = -(1+t) & \text{regulär} \\ \tilde{p}_2(t) = \frac{1}{t^2} = \frac{\tilde{a}_2(t)}{t^2} & \text{mit } \tilde{a}_2(t) = 1 & \text{regulär}\end{array}$$

$\tilde{a}_1$ 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

$$\begin{aligned}&t^2 \textstyle\sum_{n=0}^{\infty} w_n(n+\sigma)(n+\sigma-1)t^{n+\sigma-2} - \\ &\quad - (t+t^2)\textstyle\sum_{n=0}^{\infty} w_n(n+\sigma)t^{n+\sigma-1} + \sum_{n=0}^{\infty} w_n t^{n+\sigma} = 0 \\ &\textstyle\sum_{n=0}^{\infty} w_n(n+\sigma)(n+\sigma-1)t^{n+\sigma} - \sum_{n=0}^{\infty} w_n(n+\sigma)t^{n+\sigma} - \\ &\quad - \textstyle\sum_{n=0}^{\infty} w_n(n+\sigma)t^{n+\sigma+1} + \sum_{n=0}^{\infty} w_n t^{n+\sigma} = 0\end{aligned}$$

Change of index: $m = n + 1$, $n = m - 1$ in the third sum yields

$$\sum_{n=0}^{\infty} w_n\Big[(n+\sigma)(n+\sigma-2) + 1\Big]t^{n+\sigma} - \sum_{m=1}^{\infty} w_{m-1}(m-1+\sigma)t^{m+\sigma} = 0.$$

In the second sum, substitute m for n

$$\sum_{n=0}^{\infty} w_n\Big[(n+\sigma)(n+\sigma-2) + 1\Big]t^{n+\sigma} - \sum_{n=1}^{\infty} w_{n-1}(n+\sigma-1)t^{n+\sigma} = 0.$$

We write out explicitly the $n = 0$ term of the first sum

$$w_0\left[\sigma(\sigma-2)+1\right]t^\sigma + \sum_{n=1}^{\infty} w_n\left[(n+\sigma)(n+\sigma-2)+1\right]t^{n+\sigma} - \\ - \sum_{n=1}^{\infty} w_{n-1}(n+\sigma-1)\,t^{n+\sigma} = 0.$$

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

$$w_0\left[\sigma(\sigma-2)+1\right] = 0, \quad (12.37)$$

$$w_n\left[(n+\sigma)(n+\sigma-2)+1\right] - w_{n-1}(n+\sigma-1) = 0. \quad (12.38)$$

ad (12.37) for w_0:

$$\begin{aligned} \sigma(\sigma-2)+1 &= 0 \\ \sigma^2 - 2\sigma + 1 &= 0 \\ (\sigma-1)^2 &= 0 \quad \Longrightarrow \sigma_\infty^{(1,2)} = 1 \end{aligned}$$

The charakteristic exponent is $\sigma_\infty^{(1)} = \sigma_\infty^{(2)} = 1$.

ad (12.38)for w_n: For the coefficients $w_n$we have the recursion formula

$$\begin{aligned} w_n\left[(n+\sigma)(n+\sigma-2)+1\right] &= w_{n-1}(n+\sigma-1) \\ \Longrightarrow w_n &= \frac{n+\sigma-1}{(n+\sigma)(n+\sigma-2)+1}w_{n-1}. \end{aligned}$$

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:

$$\begin{aligned} w_0 &= 1 = \frac{1}{1} = \frac{1}{0!} \\ w_1 &= \frac{1}{1} = \frac{1}{1!} \\ w_2 &= \frac{1}{1\cdot 2} = \frac{1}{2!} \\ w_3 &= \frac{1}{1\cdot 2\cdot 3} = \frac{1}{3!} \\ &\vdots \\ w_n &= \frac{1}{1\cdot 2\cdot 3\cdot\cdots\cdot n} = \frac{1}{n!} \end{aligned}$$

And finally,

$$u_1(t) = t^\sigma \sum_{n=0}^{\infty} w_n t^n = t\sum_{n=0}^{\infty}\frac{t^n}{n!} = te^t.$$

- Notice that both characteristic exponents are equal; hence we have to employ the d'Alambert 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 $\tilde{p}_1$ ein,

$$\begin{aligned} u_1(t) &= te^t \\ u_1'(t) &= e^t(1+t) \\ \tilde{p}_1(t) &= -\left(\frac{1}{t}+1\right), \end{aligned}$$

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

$$u_2(t) = te^t \int_0^t \frac{1}{t}e^{-t}dt.$$

- Therefore, with $t = \frac{1}{z}$, $u(t) = w(z)$, the two linear independent solutions around the regular singular point at $z = \infty$ are

$$w_1(z) = \frac{1}{z}\exp\left(\frac{1}{z}\right), \text{ and}$$

$$w_2(z) \quad = \quad \frac{1}{z}\exp\left(\frac{1}{z}\right)\int_0^{\frac{1}{z}}\frac{1}{t}e^{-t}dt.$$

12.4 Hypergeometric function

12.4.1 Definition

A *hypergeometric series* is a series

$$\sum_{j=0}^{\infty} c_j, \tag{12.39}$$

with c_{j+1}/c_j is a *rational function* of j, so that it can be factorized by

$$\frac{c_{j+1}}{c_j} = \frac{(j+a_1)(j+a_2)\cdots(j+a_p)}{(j+b_1)(j+b_2)\cdots(j+b_q)}\frac{x}{j+1}. \tag{12.40}$$

The factor $j+1$ in the denominator has been chosen to define the fachtor $j!$ in the definition below; if it does not arise "naturally" we may just obtain it by compensating it with the factor $j+1$ in the numerator. With this ratio, the hypergeometric series (12.39) can be written i terms of *shifted factorials*, or, by another naming, the *Pochhammer symbol*, as

$$\begin{aligned}
&\textstyle\sum_{j=0}^{\infty} c_j \\
&\quad = c_0 \textstyle\sum_{j=0}^{\infty} \frac{(a_1)_j (a_2)_j \cdots (a_p)_j}{(b_1)_j (b_2)_j \cdots (b_q)_j}\frac{x^j}{j!} \\
&\quad = c_0\, {}_pF_q\left(\begin{matrix} a_1,\ldots,a_p \\ b_1,\ldots,b_p \end{matrix}; x\right), \text{ or} \\
&\quad = c_0\, {}_pF_q\left(a_1,\ldots,a_p; b_1,\ldots,b_p; x\right).
\end{aligned} \tag{12.41}$$

Apart from this definition *via* hypergeometric series, the Gauss *hypergeometric function*, or, used synonymuously, the *Gauss series*

$$\begin{aligned}
&{}_2F_1\left(\begin{matrix} a,b \\ c \end{matrix}; x\right) = {}_2F_1\left(a,b;c;x\right) = \textstyle\sum_{j=0}^{\infty} \frac{(a)_j (b)_j}{(c)_j}\frac{x^j}{j!} \\
&\quad = 1 + \frac{ab}{c}x + \frac{1}{2!}\frac{a(a+1)b(b+1)}{c(c+1)}x^2
\end{aligned} \tag{12.42}$$

can be defined as a solution of a *Fuchsian differential equation* which has at most *three regular singularities* at 0, 1, and ∞.

Indeed, any Fuchsian equation with finite regular singularities at x_1 and x_2 can be rewritten into the Gaussian form with regular singularities at 0, 1, and ∞. This can be demonstrated by rewriting any such equation of the form

The Bessel equation has a regular singular point at 0, and an irregular singular point at infinity.

$$\begin{aligned}
&w''(x) + \left(\frac{A_1}{x-x_1} + \frac{A_2}{x-x_2}\right)w'(x) \\
&\quad + \left(\frac{B_1}{(x-x_1)^2} + \frac{B_2}{(x-x_2)^2} + \frac{C_1}{x-x_1} + \frac{C_2}{x-x_2}\right)w(x) = 0
\end{aligned} \tag{12.43}$$

through transforming Eq. (12.43) into the *hypergeometric equation*

$$\left[\frac{d^2}{dx^2} + \frac{(a+b+1)x-c}{x(x-1)}\frac{d}{dx} + \frac{ab}{x(x-1)}\right] {}_2F_1(a,b;c;x) = 0, \tag{12.44}$$

where the solution is proportional to the Gauss hypergeometric function

$$w(x) \longrightarrow (x-x_1)^{\sigma_1^{(1)}}(x-x_2)^{\sigma_2^{(2)}}\ {}_2F_1(a,b;c;x), \tag{12.45}$$

and the variable transform as

$$\begin{aligned} &x \longrightarrow x = \tfrac{x-x_1}{x_2-x_1}, \text{ with}\\ &a = \sigma_1^{(1)}+\sigma_2^{(1)}+\sigma_\infty^{(1)},\\ &b = \sigma_1^{(1)}+\sigma_2^{(1)}+\sigma_\infty^{(2)},\\ &c = 1+\sigma_1^{(1)}-\sigma_1^{(2)}. \end{aligned} \tag{12.46}$$

where $\sigma_j^{(i)}$ stands for the ith characteristic exponent of the jth singularity.

Whereas the full transformation from Eq. (12.43) to the hypergeometric equation (12.44) will not been given, we shall show that the Gauss hypergeometric function ${}_2F_1$ satisfies the hypergeometric equation (12.44).

First, define the differential operator

$$\vartheta = x\frac{d}{dx}, \tag{12.47}$$

and observe that

$$\begin{aligned} \vartheta(\vartheta+c-1)x^n &= x\tfrac{d}{dx}\left(x\tfrac{d}{dx}+c-1\right)x^n\\ &= x\tfrac{d}{dx}\left(xnx^{n-1}+cx^n-x^n\right)\\ &= x\tfrac{d}{dx}\left(nx^n+cx^n-x^n\right)\\ &= x\tfrac{d}{dx}\left(n+c-1\right)x^n\\ &= n\left(n+c-1\right)x^n. \end{aligned} \tag{12.48}$$

Thus, if we apply $\vartheta(\vartheta+c-1)$ to ${}_2F_1$, then

$$\begin{aligned} &\vartheta(\vartheta+c-1)\,{}_2F_1(a,b;c;x)\\ &\quad= \vartheta(\vartheta+c-1)\sum_{j=0}^\infty \tfrac{(a)_j(b)_j}{(c)_j}\tfrac{x^j}{j!}\\ &\quad= \sum_{j=0}^\infty \tfrac{(a)_j(b)_j}{(c)_j}\tfrac{j(j+c-1)x^j}{j!}\\ &\quad= \sum_{j=1}^\infty \tfrac{(a)_j(b)_j}{(c)_j}\tfrac{j(j+c-1)x^j}{j!}\\ &\quad= \sum_{j=1}^\infty \tfrac{(a)_j(b)_j}{(c)_j}\tfrac{(j+c-1)x^j}{(j-1)!}\\ &\quad[\text{index shift: } j\to n+1, n=j-1, n\ge 0]\\ &\quad= \sum_{n=0}^\infty \tfrac{(a)_{n+1}(b)_{n+1}}{(c)_{n+1}}\tfrac{(n+1+c-1)x^{n+1}}{n!}\\ &\quad= x\sum_{n=0}^\infty \tfrac{(a)_n(a+n)(b)_n(b+n)}{(c)_n(c+n)}\tfrac{(n+c)x^n}{n!}\\ &\quad= x\sum_{n=0}^\infty \tfrac{(a)_n(b)_n}{(c)_n}\tfrac{(a+n)(b+n)x^n}{n!}\\ &\quad= x(\vartheta+a)(\vartheta+b)\sum_{n=0}^\infty \tfrac{(a)_n(b)_n}{(c)_n}\tfrac{x^n}{n!}\\ &\quad= x(\vartheta+a)(\vartheta+b)\,{}_2F_1(a,b;c;x), \end{aligned} \tag{12.49}$$

where we have used that

$$(a)_{n+1} = a(a+1)\cdots(a+n-1)(a+n) = (a)_n(a+n). \tag{12.50}$$

Writing out ϑ in Eq. (12.49) explicitly yields

$$\begin{aligned}
&\{\vartheta(\vartheta+c-1)-x(\vartheta+a)(\vartheta+b)\}\,{}_2F_1(a,b;c;x)=0,\\
&\left\{x\frac{d}{dx}\left(x\frac{d}{dx}+c-1\right)-x\left(x\frac{d}{dx}+a\right)\left(x\frac{d}{dx}+b\right)\right\}{}_2F_1(a,b;c;x)=0,\\
&\left\{\frac{d}{dx}\left(x\frac{d}{dx}+c-1\right)-\left(x\frac{d}{dx}+a\right)\left(x\frac{d}{dx}+b\right)\right\}{}_2F_1(a,b;c;x)=0,\\
&\left\{\frac{d}{dx}+x\frac{d^2}{dx^2}+(c-1)\frac{d}{dx}-\left(x^2\frac{d^2}{dx^2}+x\frac{d}{dx}+bx\frac{d}{dx}+ax\frac{d}{dx}+ab\right)\right\}{}_2F_1(a,b;c;x)=0,\\
&\left\{\left(x-x^2\right)\frac{d^2}{dx^2}+(1+c-1-x-x(a+b))\frac{d}{dx}+ab\right\}{}_2F_1(a,b;c;x)=0,\\
&\left\{-(x(x-1))\frac{d^2}{dx^2}-(c-x(1+a+b))\frac{d}{dx}-ab\right\}{}_2F_1(a,b;c;x)=0,\\
&\left\{\frac{d^2}{dx^2}+\frac{x(1+a+b)-c}{x(x-1)}\frac{d}{dx}+\frac{ab}{x(x-1)}\right\}{}_2F_1(a,b;c;x)=0.
\end{aligned} \tag{12.51}$$

12.4.2 *Properties*

There exist many properties of the hypergeometric series. In the following we shall mention a few.

$$\frac{d}{dz}\,{}_2F_1(a,b;c;z)=\frac{ab}{c}\,{}_2F_1(a+1,b+1,c+1;z). \tag{12.52}$$

$$\begin{aligned}
\frac{d}{dz}\,{}_2F_1(a,b,c;z) &= \frac{d}{dz}\sum_{n=0}^{\infty}\frac{(a)_n(b)_n}{(c)_n}\frac{z^n}{n!}=\\
&= \sum_{n=0}^{\infty}\frac{(a)_n(b)_n}{(c)_n}n\frac{z^{n-1}}{n!}\\
&= \sum_{n=1}^{\infty}\frac{(a)_n(b)_n}{(c)_n}\frac{z^{n-1}}{(n-1)!}
\end{aligned}$$

Index shift $n\to n+1$, $m=n-1$:

$$\frac{d}{dz}\,{}_2F_1(a,b;c;z)=\sum_{n=0}^{\infty}\frac{(a)_{n+1}(b)_{n+1}}{(c)_{n+1}}\frac{z^n}{n!}$$

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:

$${}_2F_1(a,b;c;x)=\frac{\Gamma(c)}{\Gamma(b)\Gamma(c-b)}\int_0^1 t^{b-1}(1-t)^{c-b-1}(1-xt)^{-a}dt. \tag{12.53}$$

For $\Re(c-a-b)>0$, we also state Gauss' theorem

$$ {}_2F_1(a,b;c;1)=\sum_{j=0}^{\infty}\frac{(a)_j(b)_j}{j!(c)_j}=\frac{\Gamma(c)\Gamma(c-a-b)}{\Gamma(c-a)\Gamma(c-b)}. \tag{12.54} $$

For a proof, we can set $x=1$ in Euler's integral representation, and the Beta function defined in Eq. (12.16).

12.4.3 Plasticity

Some of the most important elementary functions can be expressed as hypergeometric series; most importantly the Gaussion one ${}_2F_1$, which is sometimes denoted by just F. Let us enumerate a few.

$$
\begin{aligned}
e^x &= {}_0F_0(-;-;x) && (12.55)\\
\cos x &= {}_0F_1(-;\frac{1}{2};-\frac{x^2}{4}) && (12.56)\\
\sin x &= x\,{}_0F_1(-;\frac{3}{2};-\frac{x^2}{4}) && (12.57)\\
(1-x)^{-a} &= {}_1F_0(a;-;x) && (12.58)\\
\sin^{-1}x &= x\,{}_2F_1(\frac{1}{2},\frac{1}{2};\frac{3}{2};x^2) && (12.59)\\
\tan^{-1}x &= x\,{}_2F_1(\frac{1}{2},1;\frac{3}{2};-x^2) && (12.60)\\
\log(1+x) &= x\,{}_2F_1(1,1;2;-x) && (12.61)\\
H_{2n}(x) &= \frac{(-1)^n(2n)!}{n!}\,{}_1F_1(-n;\frac{1}{2};x^2) && (12.62)\\
H_{2n+1}(x) &= 2x\frac{(-1)^n(2n+1)!}{n!}\,{}_1F_1(-n;\frac{3}{2};x^2) && (12.63)\\
L_n^{\alpha}(x) &= \begin{pmatrix} n+\alpha \\ n \end{pmatrix}{}_1F_1(-n;\alpha+1;x) && (12.64)\\
P_n(x) &= P_n^{(0,0)}(x)={}_2F_1(-n,n+1;1;\frac{1-x}{2}), && (12.65)\\
C_n^{\gamma}(x) &= \frac{(2\gamma)_n}{\left(\gamma+\frac{1}{2}\right)_n}P_n^{(\gamma-\frac{1}{2},\gamma-\frac{1}{2})}(x), && (12.66)\\
T_n(x) &= \frac{n!}{\left(\frac{1}{2}\right)_n}P_n^{(-\frac{1}{2},-\frac{1}{2})}(x), && (12.67)\\
J_{\alpha}(x) &= \frac{\left(\frac{x}{2}\right)^{\alpha}}{\Gamma(\alpha+1)}\,{}_0F_1(-;\alpha+1;-\frac{1}{4}x^2), && (12.68)
\end{aligned}
$$

where H stands for *Hermite polynomials*, L for *Laguerre polynomials*,

$$ P_n^{(\alpha,\beta)}(x)=\frac{(\alpha+1)_n}{n!}\,{}_2F_1(-n,n+\alpha+\beta+1;\alpha+1;\frac{1-x}{2}) \tag{12.69} $$

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

$$ {}_2F_1(1,1,2;z) = \sum_{m=0}^{\infty} \frac{[(1)_m]^2}{(2)_m}\frac{z^m}{m!} = \sum_{m=0}^{\infty} \frac{[1\cdot 2\cdot \cdots \cdot m]^2}{2\cdot(2+1)\cdot\cdots\cdot(2+m-1)}\frac{z^m}{m!} $$

With

$$ (1)_m = 1\cdot 2\cdot\cdots\cdot m = m!, \qquad (2)_m = 2\cdot(2+1)\cdot\cdots\cdot(2+m-1) = (m+1)! $$

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

$$ \log(1+x) = \sum_{k=1}^{\infty} (-1)^{k+1}\frac{x^k}{k} \qquad \text{für} \quad -1 < x \le 1 $$

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$n \ge 0$ the series stops after a finite number of terms, because the factor $-n+i-1 = 0$ für $i = n+1$ 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,

$$ \begin{aligned} (2m)! &= 1\cdot 2\cdot 3\cdot\cdots\cdot(2m-1)(2m)=(2m-1)!!(2m)!!= \\ &= 1\cdot 3\cdot 5\cdot\cdots\cdot(2m-1)\cdot 2\cdot 4\cdot 6\cdot\cdots\cdot(2m)= \\ &= \left(\frac{1}{2}\right)_m 2^m\cdot 2^m m!=2^{2m}m!\left(\frac{1}{2}\right)_m \Longrightarrow \left(\frac{1}{2}\right)_m=\frac{(2m)!}{2^{2m}m!} \end{aligned} $$

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

$$ \sin z F\left(\frac{1}{2},\frac{1}{2},\frac{3}{2};\sin^2 z\right)=\arcsin(\sin z)=z. $$

12.4.4 Four forms

We state without proof the four forms of Gauss' hypergeometric function [5].

$$
\begin{aligned}
F(a,b;c;x) &= (1-x)^{c-a-b}F(c-a,c-b;c;x) && (12.70)\\
&= (1-x)^{-a}F\left(a,c-b;c;\frac{x}{x-1}\right) && (12.71)\\
&= (1-x)^{-b}F\left(b,c-a;c;\frac{x}{x-1}\right). && (12.72)
\end{aligned}
$$

[5] 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

12.5 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 [6]. We have already encountered at least two such prospective bases [cf. Eq. (7.2)]:

$$
\begin{aligned}
&\{1,x,x^2,\ldots,x_k,\ldots\} \text{ with } f(x)=\textstyle\sum_{k=0}^{\infty} c_k x^k,\\
&\left\{e^{ikx}\mid k\in\mathbb{Z}\right\} \quad \text{for } f(x+2\pi)=f(x)\\
&\qquad \text{with } f(x)=\textstyle\sum_{k=-\infty}^{\infty} c_k e^{ikx},\\
&\qquad \text{where } c_k=\tfrac{1}{2\pi}\textstyle\int_{-\pi}^{\pi} f(x)e^{-ikx}dx.
\end{aligned}
\qquad (12.73)
$$

[6] 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. 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

In particular, there exist systems of orthogonal functions of that kind. In order to claim this, 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* of two real-valued functions $f(x)$ and $g(x)$ by the integral [7]

$$\langle f \mid g\rangle = \int_a^b f(x)g(x)\rho(x)dx \qquad (12.74)$$

[7] 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

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 $\langle f \mid g\rangle$ satisfies all requirements of a scalar product. A system of functions $\{\psi_0,\psi_1,\psi_2,\ldots,\psi_k,\ldots\}$ is orthogonal if

$$\langle \psi_j \mid \psi_k\rangle = \int_a^b \psi_j(x)\psi_k(x)\rho(x)dx=\delta_{jk}. \qquad (12.75)$$

Suppose, in some generality, that $\{f_0,f_1,f_2,\ldots,f_k,\ldots\}$ is a sequence of nonorthogonal functions. Then we can apply a *Gram-Schmidt orthogonalization process* to these functions and thereby obtain orthogonal functions $\{\phi_0,\phi_1,\phi_2,\ldots,\phi_k,\ldots\}$ by

$$
\begin{aligned}
&\phi_0(x)=f_0(x),\\
&\phi_k(x)=f_k(x)-\textstyle\sum_{j=0}^{k-1}\frac{\langle f_k|\phi_j\rangle}{\langle \phi_j|\phi_j\rangle}\phi_j(x).
\end{aligned}
\qquad (12.76)
$$

Note that the proof of the Gram-Schmidt process in the functional context is analoguous to the one in the vector context.

12.6 Legendre polynomials

The system of polynomial functions $\{1, x, x^2, \ldots, x_k, \ldots\}$ is such a non orthogonal sequence in this sense, as, for instance, with $\rho = 1$ and $b = -a = 1$,

$$\langle 1 \mid x^2 \rangle = \int_{a=-1}^{b=1} x^2 dx = \frac{b^3 - a^3}{3} = \frac{2}{3}. \tag{12.77}$$

Hence, by the Gram-Schmidt process we obtain

$$\begin{aligned}
\phi_0(x) &= 1, \\
\phi_1(x) &= x - \tfrac{\langle x|1\rangle}{\langle 1|1\rangle} 1 \\
&= x - 0 = x, \\
\phi_2(x) &= x^2 - \tfrac{\langle x^2|1\rangle}{\langle 1|1\rangle} 1 - \tfrac{\langle x^2|x\rangle}{\langle x|x\rangle} x \\
&= x^2 - \tfrac{2/3}{2} 1 - 0x = x^2 - \tfrac{1}{3}, \\
&\vdots
\end{aligned} \tag{12.78}$$

If we are "forcing" a "normalization" of

$$\phi_k(1) = 1, \tag{12.79}$$

then this system of orthogonal polynomials is the classical *Legendre polynomials*

$$\begin{aligned}
P_0(x) &= 1, \\
P_1(x) &= x, \\
P_2(x) &= \left(x^2 - \tfrac{1}{3}\right) / \tfrac{2}{3} = \tfrac{1}{2}\left(3x^2 - 1\right), \\
&\vdots
\end{aligned} \tag{12.80}$$

Why should we be interested in orthonormal systems of functions? Because, as pointed out earlier, they could be 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*

$$(x^2 - 1)[P_l(x)]'' + 2x[P_l(x)]' = l(l+1)P_l(x), \text{ for } l \in \mathbb{N}_0 \tag{12.81}$$

whose Sturm-Liouville form has been mentioned earlier in Table 10.1 on page 161. For a proof, we refer to the literature.

12.6.1 Rodrigues formula

We just state the Rodrigues formula for Legendre polynomials

$$P_l(x) = \frac{1}{2^l l!} \frac{d^l}{dx^l} (x^2 - 1)^l, \text{ for } l \in \mathbb{N}_0. \tag{12.82}$$

without proof.

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, $P_l(-x) = (-1)^l P_l(x)$. Moreover, $P_l(-1) = (-1)^l$ and $P_{2k+1}(0) = 0$.

This can be shown by the substitution $t = -x$, $dt = -dx$, and insertion into the Rodrigues formula:

$$\begin{aligned} P_l(-x) &= \frac{1}{2^l l!}\frac{d^l}{du^l}(u^2-1)^l\Big|_{u=-x} = [u \to -u] = \\ &= \frac{1}{(-1)^l}\frac{1}{2^l l!}\frac{d^l}{du^l}(u^2-1)^l\Big|_{u=x} = (-1)^l P_l(x). \end{aligned}$$

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.

12.6.2 *Generating function*

For $|x| < 1$ and $|1| < 1$ the Legendre polynomials have the following generating function

$$g(x,t) = \frac{1}{\sqrt{1-2xt+t^2}} = \sum_{l=0}^{\infty} t^l P_l(x). \tag{12.83}$$

No proof is given here.

12.6.3 *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 $l = 1, 2, \ldots$, the three term recursion formula

$$(2l+1)xP_l(x) = (l+1)P_{l+1}(x) + lP_{l-1}(x), \tag{12.84}$$

or, by substituting $l-1$ for l, for $l = 2, 3\ldots$,

$$(2l-1)xP_{l-1}(x) = lP_l(x) + (l-1)P_{l-2}(x), \tag{12.85}$$

can be proven as follows.

$$\begin{aligned} g(x,t) &= \frac{1}{\sqrt{1-2tx+t^2}} = \sum_{n=0}^{\infty} t^n P_n(x) \\ \frac{\partial}{\partial t} g(x,t) &= -\frac{1}{2}(1-2tx+t^2)^{-\frac{3}{2}}(-2x+2t) = \frac{1}{\sqrt{1-2tx+t^2}}\frac{x-t}{1-2tx+t^2} \\ \frac{\partial}{\partial t} g(x,t) &= \frac{x-t}{1-2tx+t^2}\sum_{n=0}^{\infty} t^n P_n(x) = \sum_{n=0}^{\infty} n t^{n-1} P_n(x) \\ (x-t)\sum_{n=0}^{\infty} t^n P_n(x) &- (1-2tx+t^2)\sum_{n=0}^{\infty} n t^{n-1} P_n(x) = 0 \end{aligned}$$

$$\sum_{n=0}^{\infty} x t^n P_n(x) - \sum_{n=0}^{\infty} t^{n+1} P_n(x) - \sum_{n=1}^{\infty} n t^{n-1} P_n(x) +$$

$$+ \sum_{n=0}^{\infty} 2xnt^n P_n(x) - \sum_{n=0}^{\infty} nt^{n+1} P_n(x) = 0$$

$$\sum_{n=0}^{\infty} (2n+1) x t^n P_n(x) - \sum_{n=0}^{\infty} (n+1) t^{n+1} P_n(x) - \sum_{n=1}^{\infty} n t^{n-1} P_n(x) = 0$$

$$\sum_{n=0}^{\infty} (2n+1) x t^n P_n(x) - \sum_{n=1}^{\infty} n t^n P_{n-1}(x) - \sum_{n=0}^{\infty} (n+1) t^n P_{n+1}(x) = 0,$$

$$xP_0(x) - P_1(x) + \sum_{n=1}^{\infty} t^n \Big[(2n+1) x P_n(x) - n P_{n-1}(x) - (n+1) P_{n+1}(x) \Big] = 0,$$

hence

$$xP_0(x) - P_1(x) = 0, \qquad (2n+1)xP_n(x) - nP_{n-1}(x) - (n+1)P_{n+1}(x) = 0,$$

hence

$$P_1(x) = xP_0(x), \qquad (n+1)P_{n+1}(x) = (2n+1)xP_n(x) - nP_{n-1}(x).$$

Let us prove

$$P_{l-1}(x) = P_l'(x) - 2xP_{l-1}'(x) + P_{l-2}'(x). \tag{12.86}$$

$$g(x,t) = \frac{1}{\sqrt{1-2tx+t^2}} = \sum_{n=0}^{\infty} t^n P_n(x)$$

$$\frac{\partial}{\partial x} g(x,t) = -\frac{1}{2}(1-2tx+t^2)^{-\frac{3}{2}}(-2t) = \frac{1}{\sqrt{1-2tx+t^2}} \, \frac{t}{1-2tx+t^2}$$

$$\frac{\partial}{\partial x} g(x,t) = \frac{t}{1-2tx+t^2} \sum_{n=0}^{\infty} t^n P_n(x) = \sum_{n=0}^{\infty} t^n P_n'(x)$$

$$\sum_{n=0}^{\infty} t^{n+1} P_n(x) = \sum_{n=0}^{\infty} t^n P_n'(x) - \sum_{n=0}^{\infty} 2xt^{n+1} P_n'(x) + \sum_{n=0}^{\infty} t^{n+2} P_n'(x)$$

$$\sum_{n=1}^{\infty} t^n P_{n-1}(x) = \sum_{n=0}^{\infty} t^n P_n'(x) - \sum_{n=1}^{\infty} 2xt^n P_{n-1}'(x) + \sum_{n=2}^{\infty} t^n P_{n-2}'(x)$$

$$tP_0 + \sum_{n=2}^{\infty} t^n P_{n-1}(x) = P_0'(x) + tP_1'(x) + \sum_{n=2}^{\infty} t^n P_n'(x) -$$

$$-2xtP_0' - \sum_{n=2}^{\infty} 2xt^n P_{n-1}'(x) + \sum_{n=2}^{\infty} t^n P_{n-2}'(x)$$

$$P_0'(x) + t\Big[P_1'(x) - P_0(x) - 2xP_0'(x)\Big] +$$

$$+ \sum_{n=2}^{\infty} t^n [P_n'(x) - 2xP_{n-1}'(x) + P_{n-2}'(x) - P_{n-1}(x)] = 0$$

$P_0'(x) = 0$, hence $P_0(x) = \text{const.}$

$$P_1'(x) - P_0(x) - 2xP_0'(x) = 0.$$

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

$$P_{l+1}'(x) - P_{l-1}'(x) = (2l+1)P_l(x). \tag{12.87}$$

$$\begin{array}{rcl} (n+1)P_{n+1}(x) & = & (2n+1)xP_n(x) - nP_{n-1}(x) \quad \Big| \dfrac{d}{dx} \\ (n+1)P_{n+1}'(x) & = & (2n+1)P_n(x) + (2n+1)xP_n'(x) - nP_{n-1}'(x) \quad \Big| \cdot 2 \\ \text{(i):} \quad (2n+2)P_{n+1}'(x) & = & 2(2n+1)P_n(x) + 2(2n+1)xP_n'(x) - 2nP_{n-1}'(x) \end{array}$$

$$P_{n+1}'(x) - 2xP_n'(x) + P_{n-1}'(x) = P_n(x) \quad \Big| \cdot (2n+1)$$

$$\text{(ii):} \quad (2n+1)P_{n+1}'(x) - 2(2n+1)xP_n'(x) + (2n+1)P_{n-1}'(x) = (2n+1)P_n(x)$$

We subtract (ii) from (i):

$$P_{n+1}'(x) + 2(2n+1)xP_n'(x) - (2n+1)P_{n-1}'(x) =$$

$$= (2n+1)P_n(x) + 2(2n+1)xP_n'(x) - 2nP_{n-1}'(x);$$

hence

$$P_{n+1}'(x) - P_{n-1}'(x) = (2n+1)P_n(x).$$

12.6.4 Expansion in Legendre polynomials

We state without proof that square integrable functions $f(x)$ can be written as series of Legendre polynomials as

$$\begin{array}{l} f(x) = \sum_{l=0}^{\infty} a_l P_l(x), \text{ with expansion coefficients} \\ \quad a_l = \frac{2l+1}{2} \int\limits_{-1}^{+1} f(x)P_l(x)dx. \end{array} \tag{12.88}$$

Let us expand the Heaviside function defined in Eq. (8.27)

$$H(x) = \begin{cases} 1 & \text{for } x \geq 0 \\ 0 & \text{for } x < 0 \end{cases} \tag{12.89}$$

in terms of Legendre polynomials.

We shall use the recursion formula $(2l+1)P_l = P'_{l+1} - P'_{l-1}$ and rewrite

$$\begin{aligned} a_l &= \frac{1}{2}\int_0^1 \left(P'_{l+1}(x) - P'_{l-1}(x)\right)dx = \frac{1}{2}\left(P_{l+1}(x) - P_{l-1}(x)\right)\Big|_{x=0}^{1} = \\ &= \frac{1}{2}\underbrace{\left[P_{l+1}(1) - P_{l-1}(1)\right]}_{\substack{= 0 \text{ because of} \\ \text{"normalization"}}} - \frac{1}{2}\left[P_{l+1}(0) - P_{l-1}(0)\right]. \end{aligned}$$

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

$$H(x) = \frac{1}{2} + \sum_{l=0}^{\infty}(-1)^l\frac{(2l)!(4l+3)}{2^{2l+2}l!(l+1)!}P_{2l+1}(x).$$

12.7 *Associated Legendre polynomial*

Associated Legendre polynomials $P_l^m(x)$ are the solutions of the *general Legendre equation*

$$\begin{aligned} &\left\{(1-x^2)\frac{d^2}{dx^2} - 2x\frac{d}{dx} + \left[l(l+1) - \frac{m^2}{1-x^2}\right]\right\}P_l^m(x) = 0, \text{ or} \\ &\frac{d}{dx}\left((1-x^2)\frac{d}{dx}P_l^m(x)\right) + \left[l(l+1) - \frac{m^2}{1-x^2}\right]P_l^m(x) = 0 \end{aligned} \tag{12.90}$$

Eq. (12.90) reduces to the Legendre equation (12.81) on page 189 for $m = 0$; hence

$$P_l^0(x) = P_l(x). \tag{12.91}$$

More generally, by differentiating m times the Legendre equation (12.81) it can be shown that

$$P_l^m(x) = (-1)^m (1-x^2)^{\frac{m}{2}} \frac{d^m}{dx^m} P_l(x). \tag{12.92}$$

By inserting $P_l(x)$ from the *Rodrigues formula* for Legendre polynomials (12.82) we obtain

$$\begin{aligned} P_l^m(x) &= (-1)^m (1-x^2)^{\frac{m}{2}} \frac{d^m}{dx^m} \frac{1}{2^l l!} \frac{d^l}{dx^l}(x^2-1)^l \\ &= \frac{(-1)^m (1-x^2)^{\frac{m}{2}}}{2^l l!} \frac{d^{m+l}}{dx^{m+l}}(x^2-1)^l. \end{aligned} \tag{12.93}$$

In terms of the Gauss hypergeometric function the associated Legendre polynomials can be generalied to arbitrary complex indices μ, λ and argument x by

$$P_\lambda^\mu(x) = \frac{1}{\Gamma(1-\mu)} \left(\frac{1+x}{1-x}\right)^{\frac{\mu}{2}} {}_2F_1\left(-\lambda, \lambda+1; 1-\mu; \frac{1-x}{2}\right). \tag{12.94}$$

No proof is given here.

12.8 *Spherical harmonics*

Let us define the *spherical harmonics* $Y_l^m(\theta,\varphi)$ by

$$Y_l^m(\theta,\varphi) = \sqrt{\frac{(2l+1)(l-m)!}{4\pi(l+m)!}} P_l^m(\cos\theta) e^{im\varphi} \text{ for } -l \le m \le l.. \tag{12.95}$$

Spherical harmonics are solutions of the differential equation

$$[\Delta + l(l+1)]\, Y_l^m(\theta,\varphi) = 0. \tag{12.96}$$

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.

12.9 *Solution of the Schrödinger equation for a hydrogen atom*

Suppose Schrödinger, in his 1926 *annus mirabilis* which seem 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, Irene and Felicie [8]), came down from the mountains or from whatever realm he was in with that woman – and handed you over some partial differential equation for the hydrogen atom – an equation

[8] Walter Moore. *Schrödinger life and thought*. Cambridge University Press, Cambridge, UK, 1989

$$\begin{aligned} &\frac{1}{2\mu}\left(\mathscr{P}_x^2 + \mathscr{P}_y^2 + \mathscr{P}_z^2\right)\psi = (E - V)\psi \text{ , or, with } V = -\frac{e^2}{4\pi\epsilon_0 r}, \\ &-\left[\frac{\hbar^2}{2\mu}\Delta + \frac{e^2}{4\pi\epsilon_0 r}\right]\psi(\mathbf{x}) = E\psi \text{ , or} \\ &\left[\Delta + \frac{2\mu}{\hbar^2}\left(\frac{e^2}{4\pi\epsilon_0 r} + E\right)\right]\psi(\mathbf{x}) = 0, \end{aligned} \tag{12.97}$$

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 [9] 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. He might also have hinted that μ, e, and ϵ_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 (12.97).

[9] 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

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 (12.97) in terms of spherical coordinates (r,θ,φ) with $x = r\sin\theta\cos\varphi$, $y = r\sin\theta\sin\varphi$, $z = r\cos\theta$, whereby θ is the polar angle in the x–z-plane measured from the z-axis, with $0 \le \theta \le \pi$, and φ is the azimuthal angle in the x–y-plane, measured from the x-axis with $0 \le \varphi < 2\pi$ (cf page 79). In terms of spherical coordinates the Laplace operator essentially "decays into" (i.e. consists addiditively of) a radial part and an angular part

$$\begin{aligned}\Delta &= \left(\frac{\partial}{\partial x}\right)^2 + \left(\frac{\partial}{\partial y}\right)^2 + \left(\frac{\partial}{\partial z}\right)^2 \\ &= \frac{1}{r^2}\left[\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)\right. \\ &\quad \left. + \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right].\end{aligned} \tag{12.98}$$

12.9.1 Separation of variables Ansatz

This can be exploited for a *separation ov variable Ansatz*, which, according to Schrödinger, should be well known (in German *sattsam bekannt*) by now (cf chapter 11.1). We thus write the solution ψ as a product of functions of separate variables

$$\psi(r,\theta,\varphi) = R(r)Y_l^m(\theta,\varphi) = R(r)\Theta(\theta)\Phi(\varphi) \tag{12.99}$$

The spherical harmonics $Y_l^m(\theta,\varphi)$ has been written already as a reminder of what has been mentioned earlier on page 194. We will come back to it later.

12.9.2 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 (12.97) in radial coordinates

$$\begin{aligned}&\left\{\frac{1}{r^2}\left[\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)\right.\right. \\ &\quad \left. + \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right] \\ &\quad \left. + \frac{2\mu}{\hbar^2}\left(\frac{e^2}{4\pi\epsilon_0 r} + E\right)\right\}\psi(r,\theta,\varphi) = 0,\end{aligned} \tag{12.100}$$

and multiplying it with r^2

$$\begin{aligned}\Big\{\tfrac{\partial}{\partial r}\left(r^2\tfrac{\partial}{\partial r}\right)+\tfrac{2\mu r^2}{\hbar^2}\left(\tfrac{e^2}{4\pi\epsilon_0 r}+E\right)\\ +\tfrac{1}{\sin\theta}\tfrac{\partial}{\partial\theta}\sin\theta\tfrac{\partial}{\partial\theta}+\tfrac{1}{\sin^2\theta}\tfrac{\partial^2}{\partial\varphi^2}\Big\}\psi(r,\theta,\varphi)=0,\end{aligned}\tag{12.101}$$

so that, after division by $\psi(r,\theta,\varphi)=Y_l^m(\theta,\varphi)$ and writing separate variables on separate sides of the equation,

$$\begin{aligned}\tfrac{1}{R(r)}\left\{\tfrac{\partial}{\partial r}\left(r^2\tfrac{\partial}{\partial r}\right)+\tfrac{2\mu r^2}{\hbar^2}\left(\tfrac{e^2}{4\pi\epsilon_0 r}+E\right)\right\}R(r)\\ =-\tfrac{1}{Y_l^m(\theta,\varphi)}\left\{\tfrac{1}{\sin\theta}\tfrac{\partial}{\partial\theta}\sin\theta\tfrac{\partial}{\partial\theta}+\tfrac{1}{\sin^2\theta}\tfrac{\partial^2}{\partial\varphi^2}\right\}Y_l^m(\theta,\varphi)\end{aligned}\tag{12.102}$$

Because the left hand side of this equation is independent of the angular variables θ and φ, and its right hand side is independent of the radius r, both sides have to be constant; say λ. Thus we obtain two differential equations for the radial and the angular part, respectively

$$\left\{\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r}+\frac{2\mu r^2}{\hbar^2}\left(\frac{e^2}{4\pi\epsilon_0 r}+E\right)\right\}R(r)=\lambda R(r),\tag{12.103}$$

and

$$\left\{\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta}+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right\}Y_l^m(\theta,\varphi)=-\lambda Y_l^m(\theta,\varphi).\tag{12.104}$$

12.9.3 Separation of the polar angle θ from the azimuthal angle φ

As already hinted in Eq. (12.133) The angular portion can still be separated by the *Ansatz* $Y_l^m(\theta,\varphi)=\Theta(\theta)\Phi(\varphi)$, because, when multiplied by $\sin^2\theta/[\Theta(\theta)\Phi(\varphi)]$, Eq. (12.104) can be rewritten as

$$\left\{\frac{\sin\theta}{\Theta(\theta)}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial\Theta(\theta)}{\partial\theta}+\lambda\sin^2\theta\right\}+\frac{1}{\Phi(\varphi)}\frac{\partial^2\Phi(\varphi)}{\partial\varphi^2}=0,\tag{12.105}$$

and hence

$$\tfrac{\sin\theta}{\Theta(\theta)}\tfrac{\partial}{\partial\theta}\sin\theta\tfrac{\partial\Theta(\theta)}{\partial\theta}+\lambda\sin^2\theta=-\tfrac{1}{\Phi(\varphi)}\tfrac{\partial^2\Phi(\varphi)}{\partial\varphi^2}=m^2,\tag{12.106}$$

where m is some constant.

12.9.4 Solution of the equation for the azimuthal angle factor $\Phi(\varphi)$

The resulting differential equation for $\Phi(\varphi)$

$$\frac{d^2\Phi(\varphi)}{d\varphi^2}=-m^2\Phi(\varphi),\tag{12.107}$$

has the general solution

$$\Phi(\varphi)=Ae^{im\varphi}+Be^{-im\varphi}.\tag{12.108}$$

As Φ must obey the periodic poundary 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

$$\Phi_m(\varphi) = Ae^{im\varphi} \tag{12.109}$$

and require that it normalized, it follows that

$$\begin{aligned}
&\int_0^{2\pi} \overline{\Phi}_m(\varphi)\Phi_m(\varphi)d\varphi \\
&\quad = \int_0^{2\pi} \overline{A}e^{-im\varphi}Ae^{im\varphi}d\varphi \\
&\quad = \int_0^{2\pi} |A|^2 d\varphi \\
&\quad = 2\pi|A|^2 \\
&\quad = 1,
\end{aligned} \tag{12.110}$$

it is consistent to set

$$A = \frac{1}{\sqrt{2\pi}}; \tag{12.111}$$

and hence,

$$\Phi_m(\varphi) = \frac{e^{im\varphi}}{\sqrt{2\pi}} \tag{12.112}$$

Note that, for different $m \neq n$,

$$\begin{aligned}
&\int_0^{2\pi} \overline{\Phi}_n(\varphi)\Phi_m(\varphi)d\varphi \\
&\quad = \int_0^{2\pi} \frac{e^{-in\varphi}}{\sqrt{2\pi}} \frac{e^{im\varphi}}{\sqrt{2\pi}} d\varphi \\
&\quad = \int_0^{2\pi} \frac{e^{i(m-n)\varphi}}{2\pi} d\varphi \\
&\quad = -\frac{ie^{i(m-n)\varphi}}{2(m-n)\pi}\Big|_0^{2\pi} \\
&\quad = 0,
\end{aligned} \tag{12.113}$$

because $m - n \in \mathbb{Z}$.

12.9.5 Solution of the equation for the polar angle factor $\Theta(\theta)$

The left hand side of Eq. (12.106) contains only the polar coordinate. Upon division by $\sin^2\theta$ we obtain

$$\begin{aligned}
&\frac{1}{\Theta(\theta)\sin\theta}\frac{d}{d\theta}\sin\theta\frac{d\Theta(\theta)}{d\theta} + \lambda = \frac{m^2}{\sin^2\theta}, \text{ or} \\
&\frac{1}{\Theta(\theta)\sin\theta}\frac{d}{d\theta}\sin\theta\frac{d\Theta(\theta)}{d\theta} - \frac{m^2}{\sin^2\theta} = -\lambda,
\end{aligned} \tag{12.114}$$

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 (12.114)

$$\begin{aligned}
&\frac{d}{dx}\sin^2\theta\frac{d\Theta(x)}{dx} = -\lambda\Theta(x), \\
&\frac{d}{dx}(1-x^2)\frac{d\Theta(x)}{dx} + \lambda\Theta(x) = 0, \\
&\left(x^2-1\right)\frac{d^2\Theta(x)}{dx^2} + 2x\frac{d\Theta(x)}{dx} = \lambda\Theta(x),
\end{aligned} \tag{12.115}$$

which is of the same form as the *Legendre equation* (12.81) mentioned on page 189.

Consider the series *Ansatz*

$$\Theta(x) = a_0 + a_1x + a_2x^2 + \cdots + a_kx^k + \cdots \tag{12.116}$$

for solving (12.115). Insertion into (12.115) and comparing the coefficients of x for equal degrees yields the recursion relation

This is actually a "shortcut" solution of the Fuchian Equation mentioned earlier.

$$\begin{aligned}
&\left(x^2-1\right)\frac{d^2}{dx^2}[a_0+a_1x+a_2x^2+\cdots+a_kx^k+\cdots]\\
&\qquad +2x\frac{d}{dx}[a_0+a_1x+a_2x^2+\cdots+a_kx^k+\cdots]\\
&\qquad =\lambda[a_0+a_1x+a_2x^2+\cdots+a_kx^k+\cdots],\\
&\left(x^2-1\right)[2a_2+\cdots+k(k-1)a_kx^{k-2}+\cdots]\\
&\qquad +[2xa_1+2x2a_2x+\cdots+2xka_kx^{k-1}+\cdots]\\
&\qquad =\lambda[a_0+a_1x+a_2x^2+\cdots+a_kx^k+\cdots],\\
&\left(x^2-1\right)[2a_2+\cdots+k(k-1)a_kx^{k-2}+\cdots]\\
&\qquad +[2a_1x+4a_2x^2+\cdots+2ka_kx^k+\cdots]\\
&\qquad =\lambda[a_0+a_1x+a_2x^2+\cdots+a_kx^k+\cdots],\\
&[2a_2x^2+\cdots+k(k-1)a_kx^k+\cdots]\\
&\qquad -[2a_2+\cdots+k(k-1)a_kx^{k-2}+\cdots]\\
&\qquad +[2a_1x+4a_2x^2+\cdots+2ka_kx^k+\cdots]\\
&\qquad =\lambda[a_0+a_1x+a_2x^2+\cdots+a_kx^k+\cdots],\\
&[2a_2x^2+\cdots+k(k-1)a_kx^k+\cdots]\\
&\qquad -[2a_2+\cdots+k(k-1)a_kx^{k-2}\\
&\qquad\quad +(k+1)ka_{k+1}x^{k-1}+(k+2)(k+1)a_{k+2}x^k+\cdots]\\
&\qquad +[2a_1x+4a_2x^2+\cdots+2ka_kx^k+\cdots]\\
&\qquad =\lambda[a_0+a_1x+a_2x^2+\cdots+a_kx^k+\cdots],
\end{aligned}\tag{12.117}$$

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),

$$\begin{aligned}
&k(k-1)a_kx^k-(k+2)(k+1)a_{k+2}x^k+2ka_kx^k-\lambda a_kx^k=0,\\
&k(k+1)a_k-(k+2)(k+1)a_{k+2}-\lambda a_k=0,\\
&a_{k+2}=a_k\frac{k(k+1)-\lambda}{(k+2)(k+1)}.
\end{aligned}\tag{12.118}$$

In order to converge also for $x=\pm 1$, and hence for $\theta=0$ and $\theta=\pi$, the sum in (12.116) has to have only *a finite number of terms.* Because if the sum would be infinite, the terms a_k, for large k, would converge to $a_k\stackrel{k\rightarrow\infty}{\longrightarrow}a_\infty$ with constant $a_\infty\neq 0$, and thus Θ would diverge as $\Theta(1)\stackrel{k\rightarrow\infty}{\approx}ka_\infty\stackrel{k\rightarrow\infty}{\longrightarrow}\infty$. That means that, in Eq. (12.118) for some $k=l\in\mathbb{N}$, the coefficient $a_{l+2}=0$ has to vanish; thus

$$\lambda=l(l+1).\tag{12.119}$$

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 dependent factor (12.114) becomes

$$\left\{\frac{d}{dx}(1-x^2)\frac{d}{dx}+l(l+1)-\frac{m^2}{1-x^2}\right\}\Theta(x)=0,\tag{12.120}$$

This is exactly the form of the general Legendre equation (12.90), whose solution is a multiple of the associated Legendre polynomial $\Theta_l^m(x)\equiv P_l^m(x)$, with $|m|\leq l$.

12.9.6 Solution of the equation for radial factor $R(r)$

The solution of the equation (12.103)

$$\begin{aligned}&\left\{\frac{d}{dr}r^2\frac{d}{dr}+\frac{2\mu r^2}{\hbar^2}\left(\frac{e^2}{4\pi\epsilon_0 r}+E\right)\right\}R(r)=l(l+1)R(r)\text{ , or}\\&-\frac{1}{R(r)}\frac{d}{dr}r^2\frac{d}{dr}R(r)+l(l+1)-\frac{2\mu e^2}{4\pi\epsilon_0\hbar^2}r=\frac{2\mu}{\hbar^2}r^2E\end{aligned} \tag{12.121}$$

for the radial factor $R(r)$ turned out to be the most difficult part for Schrödinger [10].

[10] Walter Moore. *Schrödinger life and thought.* Cambridge University Press, Cambridge, UK, 1989

Note that, since the additive term $l(l+1)$ in (12.121) is dimensionless, 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*

$$a_0 = \frac{4\pi\epsilon_0\hbar^2}{m_e e^2} \approx 5\,10^{-11} m, \tag{12.122}$$

thereby assuming that the reduced mass is equal to the electron mass $\mu \approx m_e$. More explicitly, $r = y\frac{4\pi\epsilon_0\hbar^2}{m_e e^2}$. Second, define $\varepsilon = E\frac{2\mu a_0^2}{\hbar^2}$.

These substitutions yield

$$\begin{aligned}&-\frac{1}{R(y)}\frac{d}{dy}y^2\frac{d}{dy}R(y)+l(l+1)-2y=y^2\varepsilon\text{, or}\\&-y^2\frac{d^2}{d^2y}R(y)-2y\frac{d}{dy}R(y)+\left[l(l+1)-2y-\varepsilon y^2\right]R(y)=0.\end{aligned} \tag{12.123}$$

Now we introduce a new function $\hat{R}$ *via*

$$R(\xi) = \xi^l e^{-\frac{1}{2}\xi}\hat{R}(\xi), \tag{12.124}$$

with $\xi = \frac{2y}{n}$ and by replacing the energy variable with $\varepsilon = -\frac{1}{n^2}$, with $n \in \mathbb{N} - 0$, so that

$$\xi\frac{d^2}{d^2\xi}\hat{R}(\xi) + [2(l+1)-\xi]\frac{d}{dy}\hat{R}(\xi) + (n-l-1)\hat{R}(\xi) = 0. \tag{12.125}$$

The discretization of n can again be motivated by requiring physical properties from the solution; in particular, convergence. Consider again a series solution *Ansatz*

$$\hat{R}(\xi) = c_0 + c_1\xi + c_2\xi^2 + \cdots + c_k\xi^k + \cdots, \tag{12.126}$$

which, when inserted into (12.123), yields

$$\begin{aligned}
&\xi \frac{d^2}{d^2\xi}[c_0 + c_1\xi + c_2\xi^2 + \cdots + c_k\xi^k + \cdots]\\
&\qquad +[2(l+1)-\xi]\frac{d}{dy}[c_0 + c_1\xi + c_2\xi^2 + \cdots + c_k\xi^k + \cdots]\\
&\qquad +(n-l-1)[c_0 + c_1\xi + c_2\xi^2 + \cdots + c_k\xi^k + \cdots]\\
&\quad = 0,\\
&\xi[2c_2 + \cdots k(k-1)c_k\xi^{k-2} + \cdots]\\
&\qquad +[2(l+1)-\xi][c_1 + 2c_2\xi + \cdots + kc_k\xi^{k-1} + \cdots]\\
&\qquad +(n-l-1)[c_0 + c_1\xi + c_2\xi^2 + \cdots + c_k\xi^k + \cdots]\\
&\quad = 0,\\
&[2c_2\xi + \cdots + k(k-1)c_k\xi^{k-1} + \cdots]\\
&\qquad +2(l+1)[c_1 + 2c_2\xi + \cdots + k + c_k\xi^{k-1} + \cdots]\\
&\qquad\quad -[c_1\xi + 2c_2\xi^2 + \cdots + kc_k\xi^k + \cdots]\\
&\qquad +(n-l-1)[c_0 + c_1\xi + c_2\xi^2 + \cdots c_k\xi^k + \cdots]\\
&\quad = 0,\\
&[2c_2\xi + \cdots + k(k-1)c_k\xi^{k-1} + k(k+1)c_{k+1}\xi^k + \cdots]\\
&\qquad +2(l+1)[c_1 + 2c_2\xi + \cdots + kc_k\xi^{k-1} + (k+1)c_{k+1}\xi^k + \cdots]\\
&\qquad\quad -[c_1\xi + 2c_2\xi^2 + \cdots + kc_k\xi^k + \cdots]\\
&\qquad +(n-l-1)[c_0 + c_1\xi + c_2\xi^2 + \cdots + c_k\xi^k + \cdots]\\
&\quad = 0,
\end{aligned} \tag{12.127}$$

so that, by comparing the coefficients of ξ^k, we obtain

$$\begin{aligned}
&k(k+1)c_{k+1}\xi^k + 2(l+1)(k+1)c_{k+1}\xi^k = kc_k\xi^k - (n-l-1)c_k\xi^k,\\
&c_{k+1}[k(k+1) + 2(l+1)(k+1)] = c_k[k-(n-l-1)],\\
&c_{k+1}(k+1)(k+2l+2) = c_k(k-n+l+1),\\
&c_{k+1} = c_k\frac{k-n+l+1}{(k+1)(k+2l+2)}.
\end{aligned} \tag{12.128}$$

The series terminates at some $l = q$ when $q = n-l-1$, or $n = q+l+1$. Since q, l, and 1 are all integers, n must be an integer as well. And since $q \geq 0$, n must be at least $l+1$, or

$$l \leq n-1. \tag{12.129}$$

Thus, we end up with an *associated Laguerre equation* of the form

$$\left\{\xi\frac{d^2}{d\xi^2} + [2(l+1)-\xi]\frac{d}{d\xi} + (n-l-1)\right\}\hat{R}(\xi) = 0, \text{ with } n \geq l+1, \text{ and } n, l \in \mathbb{Z}. \tag{12.130}$$

Its solutions are the *associated Laguerre polynomials* L_{n+l}^{2l+1} which are the the $(2l+1)$-th derivatives of the Laguerre's polynomials L_{n+l}^{2l+1}; that is,

$$\begin{aligned}
L_n(x) &= e^x\frac{d^n}{dx^n}\left(x^n e^{-x}\right),\\
L_n^m(x) &= \frac{d^m}{dx^m}L_n(x).
\end{aligned} \tag{12.131}$$

This yields a normalized wave function

$$\begin{aligned}
&R_n(r) = \mathcal{N}\left(\frac{2r}{na_0}\right)^l e^{-\frac{r}{a_0 n}} L_{n+l}^{2l+1}\left(\frac{2r}{na_0}\right), \text{ with}\\
&\mathcal{N} = -\frac{2}{n^2}\sqrt{\frac{(n-l-1)!}{[(n+l)!a_0]^3}},
\end{aligned} \tag{12.132}$$

where $\mathcal{N}$ stands for the normalization factor.

12.9.7 Composition of the general solution of the Schrödinger Equation

Now we shall coagulate and combine the factorized solutions (12.133) into a complete solution of the Schrödinger equation

Always remember the alchemic principle of *solve et coagula*!

$$\begin{aligned}
&\psi_{n,l,m}(r,\theta,\varphi)\\
&\quad = R_n(r)\,Y_l^m(\theta,\varphi)\\
&\quad = R_n(r)\Theta_l^m(\theta)\Phi_m(\varphi)\\
&\quad = -\frac{2}{n^2}\sqrt{\frac{(n-l-1)!}{[(n+l)!a_0]^3}}\left(\frac{2r}{na_0}\right)^l e^{-\frac{r}{a_0 n}}\,L_{n+l}^{2l+1}\left(\frac{2r}{na_0}\right)P_l^m(x)\,\frac{e^{im\varphi}}{\sqrt{2\pi}}.
\end{aligned} \tag{12.133}$$

13
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" [1]. Unfortunately such series occur very often in physical situation; for instance in celestial mechanics or in quantum field theory, and one may wonder with Abel why, *"for the most part, it is true that the results are correct, which is very strange"* [2].

[1] Godfrey Harold Hardy. *Divergent Series*. Oxford University Press, 1949

[2] Christiane Rousseau. Divergent series: Past, present, future .... preprint, 2004. URL http://www.dms.umontreal.ca/~rousseac/divergent.pdf

13.1 Convergence and divergence

Let us first define *convergence* in the context of series. A series

$$\sum_{j=0}^{\infty} a_j = a_0 + a_1 + a_2 + \cdots \tag{13.1}$$

is said to converge to the *sum* s, if the *partial sum*

$$s_n = \sum_{j=0}^{n} a_j = a_0 + a_1 + a_2 + \cdots + a_n \tag{13.2}$$

tends to a finite limit s when $n \to \infty$; otherwise it is said to be divergent.

One of the most prominent series is the Leibniz series [3]

$$s = \sum_{j=0}^{\infty} (-1)^j = 1 - 1 + 1 - 1 + 1 - \cdots, \tag{13.3}$$

which is a particular case $q = -1$ of a *geometric series*

$$s = \sum_{j=0}^{\infty} q^j = 1 + q + q^2 + q^3 + \cdots = 1 + qs \tag{13.4}$$

which, since $s = 1 + qs$, converges to $s = 1/(1-q)$ if $|q| < 1$. Another one is

$$s = \sum_{j=0}^{\infty} (-1)^{j+1} j = 1 - 2 + 3 - 4 + 5 - \cdots = \left(\sum_{j=0}^{\infty} (-1)^j\right)\left(\sum_{k=0}^{\infty} (-1)^k\right), \tag{13.5}$$

which, in the same sense as the Leibnitz series is $1/[1-(-1)] = 1/2$, sums up to $1/4$.

[3] 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=TUkJAAAAQAAJ; 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 104 in the AMS Surveys and Monographs series*. American mathematical Society, Providence, RI, 2003

13.2 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 an 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*

$$\left(x^2\frac{d}{dx}+1\right)y(x)=x,\text{ or }\left(\frac{d}{dx}+\frac{1}{x^2}\right)y(x)=\frac{1}{x}. \tag{13.6}$$

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

$$y_s(x)=\sum_{j=0}^{\infty}(-1)^j j!x^{j+1}. \tag{13.7}$$

That (13.7) solves (13.6) can be seen by inserting the former into the latter; that is,

$$\begin{aligned}
&\left(x^2\frac{d}{dx}+1\right)\sum_{j=0}^{\infty}(-1)^j j!x^{j+1}=x,\\
&\sum_{j=0}^{\infty}(-1)^j(j+1)!x^{j+2}+\sum_{j=0}^{\infty}(-1)^j j!x^{j+1}=x,\\
&\qquad[\text{change of variable in the first sum: } j\to j-1\,]\\
&\sum_{j=1}^{\infty}(-1)^{j-1}(j+1-1)!x^{j+2-1}+\sum_{j=0}^{\infty}(-1)^j j!x^{j+1}=x,\\
&\sum_{j=1}^{\infty}(-1)^{j-1}j!x^{j+1}+x+\sum_{j=1}^{\infty}(-1)^j j!x^{j+1}=x,\\
&x+\sum_{j=1}^{\infty}(-1)^j\left[(-1)^{-1}+1\right]j!x^{j+1}=x,\\
&x+\sum_{j=1}^{\infty}(-1)^j[-1+1]\,j!x^{j+1}=x,\\
&x=x.
\end{aligned} \tag{13.8}$$

On the other hand, an exact solution can be found by *quadrature;* that is, by explicit integration (see, for instance, Chapter one of Ref. [4]). Consider the homogenuous first order differential equation

$$\left(\frac{d}{dx}+p(x)\right)y(x)=0,\text{ or }\frac{dy(x)}{dx}=-p(x)y(x),\text{ or }\frac{dy(x)}{y(x)}=-p(x)dx. \tag{13.9}$$

Integrating both sides yields

$$\log|y(x)|=-\int p(x)dx+C,\text{ or}|y(x)|=Ke^{-\int p(x)dx}, \tag{13.10}$$

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

[4] 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,

$$\begin{aligned}\frac{d}{dx}y(x)e^{P(x)} &= e^{P(x)}\frac{dy(x)}{dx}+y(x)\frac{d}{dx}e^{P(x)}\\ &= e^{P(x)}\frac{dy(x)}{dx}+y(x)p(x)e^{P(x)}\\ &= e^{P(x)}\left(\frac{d}{dx}+p(x)\right)y(x)\\ &= 0\end{aligned} \tag{13.11}$$

if and, since $e^{P(x)}\neq 0$, only if $y(x)$ satisfies the homogenuous equation (13.9). Hence,

$$\begin{aligned}&y(x)=ce^{-\int p(x)dx} \text{ is the solution of}\\ &\left(\frac{d}{dx}+p(x)\right)y(x)=0\end{aligned} \tag{13.12}$$

for some constant c.

Similarly, we can again find a solution to the inhomogenuos first order differential equation

$$\begin{aligned}&\left(\frac{d}{dx}+p(x)\right)y(x)+q(x)=0, \text{ or}\\ &\left(\frac{d}{dx}+p(x)\right)y(x)=-q(x)\end{aligned} \tag{13.13}$$

by differentiating the function $y(x)e^{P(x)}=y(x)e^{\int p(x)dx}$; that is,

$$\begin{aligned}\frac{d}{dx}y(x)e^{\int p(x)dx} &= e^{\int p(x)dx}\frac{d}{dx}y(x)+p(x)e^{\int p(x)dx}y(x)\\ &= e^{\int p(x)dx}\left(\frac{d}{dx}+p(x)\right)y(x) \qquad -e^{\int p(x)dx}q(x).\end{aligned} \tag{13.14}$$

Hence, for some constant y_0 and some a, we must have, by integration,

$$\begin{aligned}&y(x)e^{\int_a^x p(t)dt}=y_0-\int_a^x e^{\int_a^t p(s)ds}q(t)dt, \text{ and whence}\\ &y(x)=y_0e^{-\int_a^x p(t)dt}-e^{-\int_a^x p(t)dt}\int_a^x e^{\int_a^t p(s)ds}q(t)dt,\end{aligned} \tag{13.15}$$

with $y(a)=y_0$.

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,

$$\begin{aligned}y(x) &= -e^{-\int_0^x \frac{dt}{t^2}}\int_0^x e^{\int_0^t \frac{ds}{s^2}}\left(-\frac{1}{t}\right)dt\\ &= e^{\frac{1}{x}}\int_0^x \frac{e^{-\frac{1}{t}}}{t}dt\\ &= e\int_0^x \frac{e^{\frac{1}{x}-\frac{1}{t}}}{t}dt.\end{aligned} \tag{13.16}$$

With the change of coordinate *Ansatz*

$$\xi=\frac{x}{z}-1,\; z=\frac{x}{1+\xi},\; dz=-\frac{x}{(1+\xi)^2}d\xi \tag{13.17}$$

the integral (13.16) can be rewritten as

$$y(x)=\int_0^\infty \frac{e^{-\frac{\xi}{x}}}{1+\xi}d\xi. \tag{13.18}$$

Note that whereas the series solution $y_s(x)$ diverges for all nonzero x, the solution $y(x)$ in (13.18) converges and is well defined for all $x\geq 0$.

Let us now estimate the absolute difference between $y_{s_k}(x)$ which represents "$y_s((x)$ truncated after the kth term" and $y(x)$; that is, let us consider

$$|y(x)-y_{s_k}(x)| = \left|\int_0^\infty \frac{e^{-\frac{\xi}{x}}}{1+\xi}d\xi - \sum_{j=0}^{k}(-1)^j j! x^{j+1}\right|. \tag{13.19}$$

It can be shown [5] that, for any $x \geq 0$ this difference can be estimated by a bound from above

$$|y(x)-y_{s_k}(x)| \leq k! x^{k+1}. \tag{13.20}$$

[5] Christiane Rousseau. Divergent series: Past, present, future .... preprint, 2004. URL http://www.dms.umontreal.ca/~rousseac/divergent.pdf

For a proof, observe that, since

$$\sum_{k=0}^{n} a_k = a_0 \frac{1-r^{n+1}}{1-r} = a_0 r \frac{1-r^n}{1-r} \tag{13.21}$$

it is true that

$$\frac{1}{1-\zeta} = \sum_k = 0^{n-1}(-1)^k \zeta^k + (-1)^n \frac{\zeta^n}{1+\zeta}. \tag{13.22}$$

Thus

$$\begin{aligned} f(x) &= \int_0^\infty \frac{e^{-\frac{\zeta}{x}}}{1-\zeta} d\zeta \\ &= \int_0^\infty e^{-\frac{\zeta}{x}} \left(\sum_k = 0^{n-1}(-1)^k \zeta^k + (-1)^n \frac{\zeta^n}{1+\zeta}\right) d\zeta \\ &= \sum_k = 0^{n-1} \int_0^\infty (-1)^k \zeta^k e^{-\frac{\zeta}{x}} d\zeta + \int_0^\infty (-1)^n \frac{\zeta^n e^{-\frac{\zeta}{x}}}{1+\zeta} d\zeta. \end{aligned} \tag{13.23}$$

Since

$$k! = \Gamma(k+1) = \int_0^\infty z^k e^{-k} dz, \tag{13.24}$$

one obtains

$$\begin{aligned} &\int_0^\infty \zeta^k e^{-\frac{\zeta}{x}} d\zeta \\ &\quad [\text{substitution: } z = \frac{\zeta}{x}, d\zeta = x dz\,] \\ &\quad = \int_0^\infty x^{k+1} z^k e^{-z} dz \\ &\quad = x^{k+1} k!, \end{aligned} \tag{13.25}$$

and hence

$$\begin{aligned} f(x) &= \sum_k = 0^{n-1} \int_0^\infty (-1)^k \zeta^k e^{-\frac{\zeta}{x}} d\zeta + \int_0^\infty (-1)^n \frac{\zeta^n e^{-\frac{\zeta}{x}}}{1+\zeta} d\zeta \\ &= \sum_k = 0^{n-1}(-1)^k x^{k+1} k! + \int_0^\infty (-1)^n \frac{\zeta^n e^{-\frac{\zeta}{x}}}{1+\zeta} d\zeta \\ &= f_n(x) + R_n(x), \end{aligned} \tag{13.26}$$

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

$$\begin{aligned} |R_n(x)| &= \int_0^\infty \frac{\zeta^n e^{-\frac{\zeta}{x}}}{1+\zeta} \\ &\leq \int_0^\infty \zeta^n e^{-\frac{\zeta}{x}} \\ &= n! x^{n+1}. \end{aligned} \tag{13.27}$$

As a result, the remainder grows with growing number of terms contributing to the sum; a characterisztic feature of divergent series (for convergent series, the remainder decreases).

Bibliography

Oliver Aberth. *Computable Analysis.* McGraw-Hill, New York, 1980.

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.

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.

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.

M. A. Al-Gwaiz. *Sturm-Liouville Theory and its Applications.* Springer, London, 2008.

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, 1967a.

A. D. Alexandrov. Mappings of spaces with families of cones and space-time transformations. *Annali di Matematica Pura ed Applicata*, 103: 229–257, 1967b.

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.

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.

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.

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.

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. Baaz. Über den allgemeinen gehalt von beweisen. In *Contributions to General Algebra*, volume 6, pages 21–29, Vienna, 1988. Hölder-Pichler-Tempsky.

L. E. Ballentine. *Quantum Mechanics*. Prentice Hall, Englewood Cliffs, NJ, 1989.

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

W. W. Bell. *Special Functions for Scientists and Engineers*. D. Van Nostrand Company Ltd, London, 1968.

Paul Benacerraf. Tasks and supertasks, and the modern Eleatics. *Journal of Philosophy*, LIX(24):765–784, 1962. URL http://www.jstor.org/stable/2023500.

Walter Benz. *Geometrische Transformationen*. BI Wissenschaftsverlag, Mannheim, 1992.

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.

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.

E. Bishop and Douglas S. Bridges. *Constructive Analysis*. Springer, Berlin, 1985.

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

H. J. Borchers and G. C. Hegerfeldt. The structure of space-time transformations. *Communications in Mathematical Physics*, 28:259–266, 1972.

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.

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.

Douglas Bridges and F. Richman. *Varieties of Constructive Mathematics*. Cambridge University Press, Cambridge, 1987.

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

Yuri Alexandrovich Brychkov and Anatolii Platonovich Prudnikov. *Handbook of special functions: derivatives, integrals, series and other formulas*. CRC/Chapman & Hall Press, Boca Raton, London, New York, 2008.

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.

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.

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.

R. A. Campos, B. E. A. Saleh, and M. 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.

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.

A. S. Davydov. *Quantum Mechanics*. Addison-Wesley, Reading, MA, 1965.

Rene Descartes. *Discours de la méthode pour bien conduire sa raison et chercher la verité 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.

Rene Descartes. *The Philosophical Writings of Descartes. Volume 1*. Cambridge University Press, Cambridge, 1985. translated by John Cottingham, Robert Stoothoff and Dugald Murdoch.

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

Hans Jörg Dirschmid. *Tensoren und Felder*. Springer, Vienna, 1996.

S. Drobot. *Real Numbers*. Prentice-Hall, Englewood Cliffs, New Jersey, 1964.

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/S0219749910006502. URL http://dx.doi.org/10.1142/S0219749910006502.

Anatolij Dvurečenskij. *Gleason's Theorem and Its Applications*. Kluwer Academic Publishers, Dordrecht, 1993.

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.

Lawrence C. Evans. *Partial differential equations. Graduate Studies in Mathematics, volume 19*. American Mathematical Society, Providence, Rhode Island, 1998.

Graham Everest, Alf van der Poorten, Igor Shparlinski, and Thomas Ward. *Recurrence sequences. Volume 104 in the AMS Surveys and Monographs series*. American mathematical Society, Providence, RI, 2003.

William Norrie Everitt. A catalogue of Sturm-Liouville differential equations. In *Sturm-Liouville Theory, Past and Present*, pages 271–331. Birkhäuser Verlag, Basel, 2005. URL http://www.math.niu.edu/SL2/papers/birk0.pdf.

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.

Richard Phillips Feynman, Robert B. Leighton, and Matthew Sands. *The Feynman Lectures on Physics. Quantum Mechanics*, volume III. Addison-Wesley, Reading, MA, 1965.

Robert French. The Banach-Tarski theorem. *The Mathematical Intelligencer*, 10:21–28, 1988. ISSN 0343-6993. DOI: 10.1007/BF03023740. URL http://dx.doi.org/10.1007/BF03023740.

Robin O. Gandy. Church's thesis and principles for mechanics. In J. Barwise, H. J. Kreisler, and K. Kunen, editors, *The Kleene Symposium. Vol. 101 of Studies in Logic and Foundations of Mathematics*, pages 123–148. North Holland, Amsterdam, 1980.

I. M. Gel'fand and G. E. Shilov. *Generalized Functions. Vol. 1: Properties and Operations.* Academic Press, New York, 1964. Translated from the Russian by Eugene Saletan.

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.

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.

I. S. Gradshteyn and I. M. Ryzhik. *Tables of Integrals, Series, and Products, 6th ed.* Academic Press, San Diego, CA, 2000.

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.

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.

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

A. Grünbaum. *Modern Science and Zeno's paradoxes.* Allen and Unwin, London, second edition, 1968.

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

Godfrey Harold Hardy. *Divergent Series*. Oxford University Press, 1949.

Hans Havlicek. *Lineare Algebra für Technische Mathematiker*. Heldermann Verlag, Lemgo, second edition, 2008.

Jim Hefferon. Linear algebra. 320-375, 2011. URL http://joshua.smcvt.edu/linalg.html/book.pdf.

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. Creative Commons Attribution-NoncommercialShare Alike 3.0 United States License.

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.

David Hilbert. Mathematical problems. *Bulletin of the American Mathematical Society*, 8(10):437–479, 1902. DOI: 10.1090/S0002-9904-1902-00923-3. URL http://dx.doi.org/10.1090/S0002-9904-1902-00923-3.

David Hilbert. Über das Unendliche. *Mathematische Annalen*, 95(1):161–190, 1926. DOI: 10.1007/BF01206605. URL http://dx.doi.org/10.1007/BF01206605.

Howard Homes and Chris Rorres. *Elementary Linear Algebra: Applications Version*. Wiley, New York, tenth edition, 2010.

Kenneth B. Howell. *Principles of Fourier analysis*. Chapman & Hall/CRC, Boca Raton, London, New York, Washington, D.C., 2001.

Klaus Jänich. *Analysis für Physiker und Ingenieure. Funktionentheorie, Differentialgleichungen, Spezielle Funktionen*. Springer, Berlin, Heidelberg, fourth edition, 2001. URL http://www.springer.com/mathematics/analysis/book/978-3-540-41985-3.

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.

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

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.

Ebergard Klingbeil. *Tensorrechnung für Ingenieure*. Bibliographisches Institut, Mannheim, 1966.

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.

Georg Kreisel. A notion of mechanistic theory. *Synthese*, 29:11–26, 1974. DOI: 10.1007/BF00484949. URL http://dx.doi.org/10.1007/BF00484949.

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.

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.

Imre Lakatos. *Philosophical Papers. 1. The Methodology of Scientific Research Programmes*. Cambridge University Press, Cambridge, 1978.

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.

Ron Larson and Bruce H. Edwards. *Calculus*. Brooks/Cole Cengage Learning, Belmont, CA, 9th edition, 2010. ISBN 978-0-547-16702-2.

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.

H. D. P. Lee. *Zeno of Elea*. Cambridge University Press, Cambridge, 1936.

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=TUkJAAAAQAAJ.

June A. Lester. Distance preserving transformations. In Francis Buekenhout, editor, *Handbook of Incidence Geometry*. Elsevier, Amsterdam, 1995.

M. J. Lighthill. *Introduction to Fourier Analysis and Generalized Functions*. Cambridge University Press, Cambridge, 1958.

Seymour Lipschutz and Marc Lipson. *Linear algebra*. Schaum's outline series. McGraw-Hill, fourth edition, 2009.

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.

Eli Maor. *Trigonometric Delights*. Princeton University Press, Princeton, 1998. URL `http://press.princeton.edu/books/maor/`.

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.

N. David Mermin. Lecture notes on quantum computation. 2002-2008. URL `http://people.ccmr.cornell.edu/~mermin/qcomp/CS483.html`.

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

A. Messiah. *Quantum Mechanics*, volume I. North-Holland, Amsterdam, 1962.

Charles N. Moore. *Summable Series and Convergence Factors*. American Mathematical Society, New York, NY, 1938.

Walter Moore. *Schrödinger life and thought*. Cambridge University Press, Cambridge, UK, 1989.

F. D. Murnaghan. *The Unitary and Rotation Groups*. Spartan Books, Washington, D.C., 1962.

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

M. A. Nielsen and I. L. Chuang. *Quantum Computation and Quantum Information*. Cambridge University Press, Cambridge, 2000.

Asher Peres. *Quantum Theory: Concepts and Methods*. Kluwer Academic Publishers, Dordrecht, 1993.

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

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.

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.

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.

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.

Michael Reed and Barry Simon. *Methods of Mathematical Physics I: Functional Analysis*. Academic Press, New York, 1972.

Michael Reed and Barry Simon. *Methods of Mathematical Physics II: Fourier Analysis, Self-Adjointness*. Academic Press, New York, 1975.

Fred Richman and Douglas Bridges. A constructive proof of Gleason's theorem. *Journal of Functional Analysis*, 162:287–312, 1999. DOI: 10.1006/jfan.1998.3372. URL http://dx.doi.org/10.1006/jfan.1998.3372.

Christiane Rousseau. Divergent series: Past, present, future .... preprint, 2004. URL http://www.dms.umontreal.ca/~rousseac/divergent.pdf.

Rudy Rucker. *Infinity and the Mind*. Birkhäuser, Boston, 1982.

Richard Mark Sainsbury. *Paradoxes*. Cambridge University Press, Cambridge, United Kingdom, third edition, 2009. ISBN 0521720796.

Dietmar A. Salamon. *Funktionentheorie*. Birkhäuser, Basel, 2012. DOI: 10.1007/978-3-0348-0169-0. URL http://dx.doi.org/10.1007/978-3-0348-0169-0. see also URL http://www.math.ethz.ch/ salamon/PREPRINTS/cxana.pdf.

Leonard I. Schiff. *Quantum Mechanics*. McGraw-Hill, New York, 1955.

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.

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.

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. 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.

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.

Erwin Schrödinger. *Nature and the Greeks*. Cambridge University Press, Cambridge, 1954.

Erwin Schrödinger. *The Interpretation of Quantum Mechanics. Dublin Seminars (1949-1955) and Other Unpublished Essays*. Ox Bow Press, Woodbridge, Connecticut, 1995.

Laurent Schwartz. *Introduction to the Theory of Distributions*. University of Toronto Press, Toronto, 1952. collected and written by Israel Halperin.

J. Schwinger. Unitary operators bases. In *Proceedings of the National Academy of Sciences (PNAS)*, volume 46, pages 570–579, 1960. DOI: 10.1073/pnas.46.4.570. URL http://dx.doi.org/10.1073/pnas.46.4.570.

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.

Raymond M. Smullyan. *What is the Name of This Book?* Prentice-Hall, Inc., Englewood Cliffs, NJ, 1992a.

Raymond M. Smullyan. *Gödel's Incompleteness Theorems*. Oxford University Press, New York, New York, 1992b.

Ernst Snapper and Robert J. Troyer. *Metric Affine Geometry*. Academic Press, New York, 1971.

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.

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/.

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.

Karl Svozil. Are simultaneous Bell measurements possible? *New Journal of Physics*, 8:39, 1–8, 2006. DOI: 10.1088/1367-2630/8/3/039. URL http://dx.doi.org/10.1088/1367-2630/8/3/039.

Alfred Tarski. Der Wahrheitsbegriff in den Sprachen der deduktiven Disziplinen. *Akademie der Wissenschaften in Wien. Mathematisch-naturwissenschaftliche Klasse, Akademischer Anzeiger*, 69:9–12, 1932.

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.

James F. Thomson. Tasks and supertasks. *Analysis*, 15:1–13, October 1954.

A. M. Turing. On computable numbers, with an application to the Entscheidungsproblem. *Proceedings of the London Mathematical Society, Series 2*, 42, 43:230–265, 544–546, 1936-7 and 1937. DOI: 10.1112/plms/s2-42.1.230, 10.1112/plms/s2-43.6.544. URL http://dx.doi.org/10.1112/plms/s2-42.1.230,http://dx.doi.org/10.1112/plms/s2-43.6.544.

John von Neumann. Über Funktionen von Funktionaloperatoren. *Annals of Mathematics*, 32:191–226, 1931. URL http://www.jstor.org/stable/1968185.

John von Neumann. *Mathematische Grundlagen der Quantenmechanik*. Springer, Berlin, 1932.

Stan Wagon. *The Banach-Tarski Paradox*. Cambridge University Press, Cambridge, 1986.

Klaus Weihrauch. *Computable Analysis. An Introduction*. Springer, Berlin, Heidelberg, 2000.

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.

Hermann Weyl. *Philosophy of Mathematics and Natural Science*. Princeton University Press, Princeton, NJ, 1949.

John Archibald Wheeler and Wojciech Hubert Zurek. *Quantum Theory and Measurement*. Princeton University Press, Princeton, NJ, 1983.

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.

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.

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.

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.

Anton Zeilinger. The message of the quantum. *Nature*, 438:743, 2005. DOI: 10.1038/438743a. URL http://dx.doi.org/10.1038/438743a.

Index