Mathematical Methods in Quantum Mechanics

With Applications to Schrödinger Operators

Gerald Teschl

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To Susanne, Simon, and Jakob

Contents

Preface

Overview

The present text was written for my course *Schrödinger Operators* held at the University of Vienna in winter 1999, summer 2002, summer 2005, and winter 2007. It gives a brief but rather self-contained introduction to the mathematical methods of quantum mechanics with a view towards applications to Schrödinger operators. The applications presented are highly selective and many important and interesting items are not touched upon.

Part 1 is a stripped down introduction to spectral theory of unbounded operators where I try to introduce only those topics which are needed for the applications later on. This has the advantage that you will (hopefully) not get drowned in results which are never used again before you get to the applications. In particular, I am not trying to present an encyclopedic reference. Nevertheless I still feel that the first part should provide a solid background covering many important results which are usually taken for granted in more advanced books and research papers.

My approach is built around the spectral theorem as the central object. Hence I try to get to it as quickly as possible. Moreover, I do not take the detour over bounded operators but I go straight for the unbounded case. In addition, existence of spectral measures is established via the Herglotz theorem rather than the Riesz representation theorem since this approach paves the way for an investigation of spectral types via boundary values of the resolvent as the spectral parameter approaches the real line.

Part 2 starts with the free Schrödinger equation and computes the free resolvent and time evolution. In addition, I discuss position, momentum, and angular momentum operators via algebraic methods. This is usually found in any physics textbook on quantum mechanics, with the only difference that I include some technical details which are typically not found there. Then there is an introduction to one-dimensional models (Sturm–Liouville operators) including generalized eigenfunction expansions (Weyl–Titchmarsh theory) and subordinacy theory from Gilbert and Pearson. These results are applied to compute the spectrum of the hydrogen atom, where again I try to provide some mathematical details not found in physics textbooks. Further topics are nondegeneracy of the ground state, spectra of atoms (the HVZ theorem), and scattering theory (the Enß method).

Prerequisites

I assume some previous experience with Hilbert spaces and bounded linear operators which should be covered in any basic course on functional analysis. However, while this assumption is reasonable for mathematics students, it might not always be for physics students. For this reason there is a preliminary chapter reviewing all necessary results (including proofs). In addition, there is an appendix (again with proofs) providing all necessary results from measure theory.

Literature

The present book is highly influenced by the four volumes of Reed and Simon [**40**]–[**43**] (see also [**14**]) and by the book by Weidmann [**60**] (an extended version of which has recently appeared in two volumes [**62**], [**63**], however, only in German). Other books with a similar scope are for example [**14**], [**15**], [**21**], [**23**], [**39**], [**48**], and [**55**]. For those who want to know more about the physical aspects, I can recommend the classical book by Thirring [**58**] and the visual guides by Thaller [**56**], [**57**]. Further information can be found in the bibliographical notes at the end.

Reader's guide

There is some intentional overlap between Chapter 0, Chapter 1, and Chapter 2. Hence, provided you have the necessary background, you can start reading in Chapter 1 or even Chapter 2. Chapters 2 and 3 are key chapters and you should study them in detail (except for Section 2.6 which can be skipped on first reading). Chapter 4 should give you an idea of how the spectral theorem is used. You should have a look at (e.g.) the first section and you can come back to the remaining ones as needed. Chapter 5 contains two key results from quantum dynamics: Stone's theorem and the RAGE theorem. In particular the RAGE theorem shows the connections between long time behavior and spectral types. Finally, Chapter 6 is again of central importance and should be studied in detail.

The chapters in the second part are mostly independent of each other except for Chapter 7, which is a prerequisite for all others except for Chapter 9.

If you are interested in one-dimensional models (Sturm–Liouville equations), Chapter 9 is all you need.

If you are interested in atoms, read Chapter 7, Chapter 10, and Chapter 11. In particular, you can skip the separation of variables (Sections 10.3 and 10.4, which require Chapter 9) method for computing the eigenvalues of the hydrogen atom, if you are happy with the fact that there are countably many which accumulate at the bottom of the continuous spectrum.

If you are interested in scattering theory, read Chapter 7, the first two sections of Chapter 10, and Chapter 12. Chapter 5 is one of the key prerequisites in this case.

Updates

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where updates, corrections, and other material may be found, including a link to material on my own web site:

`http://www.mat.univie.ac.at/~gerald/ftp/book-schroe/`

Acknowledgments

I would like to thank Volker Enß for making his lecture notes [**18**] available to me. Many colleagues and students have made useful suggestions and pointed out mistakes in earlier drafts of this book, in particular: Kerstin Ammann, Jörg Arnberger, Chris Davis, Fritz Gesztesy, Maria Hoffmann-Ostenhof, Zhenyou Huang, Helge Krüger, Katrin Grunert, Wang Lanning, Daniel Lenz, Christine Pfeuffer, Roland Möws, Arnold L. Neidhardt, Harald

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If you also find an error or if you have comments or suggestions (no matter how small), please let me know.

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Bibliographical notes

The aim of this section is not to give a comprehensive guide to the literature, but to document the sources from which I have learned the materials and which I have used during the preparation of this text. In addition, I will point out some standard references for further reading. In some sense all books on this topic are inspired by von Neumann's celebrated monograph [**64**] and the present text is no exception.

General references for the first part are Akhiezer and Glazman [**2**], Berthier (Boutet de Monvel) [**9**], Blank, Exner, and Havlíček [**10**], Edmunds and Evans [**16**], Lax [**25**], Reed and Simon [**40**], Weidmann [**60**], [**62**], or Yosida [**66**].

Chapter 0: A first look at Banach and Hilbert spaces

As a reference for general background I can warmly recommend Kelly's classical book [**26**]. The rest is standard material and can be found in any book on functional analysis.

Chapter 1: Hilbert spaces

The material in this chapter is again classical and can be found in any book on functional analysis. I mainly follow Reed and Simon [**40**], respectively, Weidmann [**60**], with the main difference being that I use orthonormal sets and their projections as the central theme from which everything else is derived. For an alternate problem based approach see Halmos' book [**22**].

Chapter 2: Self-adjointness and spectrum

This chapter is still similar in spirit to [**40**], [**60**] with some ideas taken from Schechter [**48**].

Chapter 3: The spectral theorem

The approach via the Herglotz representation theorem follows Weidmann [**60**]. However, I use projection-valued measures as in Reed and Simon [**40**] rather than the resolution of the identity. Moreover, I have augmented the discussion by adding material on spectral types and the connections with the boundary values of the resolvent. For a survey containing several recent results see [**28**].

Chapter 4: Applications of the spectral theorem

This chapter collects several applications from various sources which I have found useful or which are needed later on. Again Reed and Simon [**40**] and Weidmann [**60**], [**63**] are the main references here.

Chapter 5: Quantum dynamics

The material is a synthesis of the lecture notes by Enß [**18**], Reed and Simon [**40**], [**42**], and Weidmann [**63**].

Chapter 6: Perturbation theory for self-adjoint operators

This chapter is similar to [**60**] (which contains more results) with the main difference that I have added some material on quadratic forms. In particular, the section on quadratic forms contains, in addition to the classical results, some material which I consider useful but was unable to find (at least not in the present form) in the literature. The prime reference here is Kato's monumental treatise [**24**] and Simon's book [**49**]. For further information on trace class operators see Simon's classic [**52**]. The idea to extend the usual notion of strong resolvent convergence by allowing the approximating operators to live on subspaces is taken from Weidmann [**62**].

Chapter 7: The free Schrödinger operator

Most of the material is classical. Much more on the Fourier transform can be found in Reed and Simon [**41**].

Chapter 8: Algebraic methods

This chapter collects some material which can be found in almost any physics text book on quantum mechanics. My only contribution is to provide some mathematical details. I recommend the classical book by Thirring [**58**] and the visual guides by Thaller [**56**], [**57**].

Chapter 9: One-dimensional Schrödinger operators

One-dimensional models have always played a central role in understanding quantum mechanical phenomena. In particular, *general wisdom used to say that Schrödinger operators should have absolutely continuous spectrum plus some discrete point spectrum, while singular continuous spectrum is a pathology that should not occur in examples with bounded V* [**14**, Sect. 10.4].

In fact, a large part of [**43**] is devoted to establishing the absence of singular continuous spectrum. This was proven wrong by Pearson, who constructed an explicit one-dimensional example with singular continuous spectrum. Moreover, after the appearance of random models, it became clear that such kind of exotic spectra (singular continuous or dense pure point) are frequently generic. The starting point is often the boundary behaviour of the Weyl m-function and its connection with the growth properties of solutions of the underlying differential equation, the latter being known as Gilbert and Pearson or subordinacy theory. One of my main goals is to give a modern introduction to this theory. The section on inverse spectral theory presents a simple proof for the Borg–Marchenko theorem (in the local version of Simon) from Bennewitz [**8**]. Again this result is the starting point of almost all other inverse spectral results for Sturm–Liouville equations and should enable the reader to start reading research papers in this area.

Other references with further information are the lecture notes by Weidmann [**61**] or the classical books by Coddington and Levinson [**13**], Levitan [**29**], Levitan and Sargsjan [**30**], [**31**], Marchenko [**33**], Naimark [**34**], Pearson [**37**]. See also the recent monographs by Rofe-Betekov and Kholkin [**46**], Zettl [**67**] or the recent collection of historic and survey articles [**4**]. For a nice introduction to random models I can recommend the recent notes by Kirsch [**27**] or the classical monographs by Carmona and Lacroix [**11**] or Pastur and Figotin [**36**]. For the discrete analog of Sturm–Liouville operators, Jacobi operators, see my monograph [**54**].

Chapter 10: One-particle Schrödinger operators

The presentation in the first two sections is influenced by Enß [**18**] and Thirring [**58**]. The solution of the Schrödinger equation in spherical coordinates can be found in any text book on quantum mechanics. Again I tried to provide some missing mathematical details. Several other explicitly solvable examples can be found in the books by Albeverio et al. [**3**] or Flügge [**19**]. For the formulation of quantum mechanics via path integrals I suggest Roepstorff [**45**] or Simon [**50**].

Chapter 11: Atomic Schrödinger operators

This chapter essentially follows Cycon, Froese, Kirsch, and Simon [**14**]. For a recent review see Simon [**51**].

Chapter 12: Scattering theory

This chapter follows the lecture notes by Enß [**18**] (see also [**17**]) using some material from Perry [**38**]. Further information on mathematical scattering theory can be found in Amrein, Jauch, and Sinha [**5**], Baumgaertel and Wollenberg [**6**], Chadan and Sabatier [**12**], Cycon, Froese, Kirsch, and Simon [**14**], Newton [**35**], Pearson [**37**], Reed and Simon [**42**], or Yafaev [**65**].

Appendix A: Almost everything about Lebesgue integration

Most parts follow Rudin's book [**47**], respectively, Bauer [**7**], with some ideas also taken from Weidmann [**60**]. I have tried to strip everything down to the results needed here while staying self-contained. Another useful reference is the book by Lieb and Loss [**32**].

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Glossary of notation

$AC(I)$	... absolutely continuous functions, 84
$\mathfrak{B}$	$= \mathfrak{B}^1$
$\mathfrak{B}^n$	... Borel σ-field of $\mathbb{R}^n$, 260
$\mathfrak{C}(\mathfrak{H})$	... set of compact operators, 128
$C(U)$	... set of continuous functions from U to $\mathbb{C}$
$C_\infty(U)$	... set of functions in $C(U)$ which vanish at ∞
$C(U,V)$	... set of continuous functions from U to V
$C_c^\infty(U,V)$	... set of compactly supported smooth functions
$\chi_\Omega(.)$	... characteristic function of the set Ω
dim	... dimension of a linear space
$\mathrm{dist}(x,Y)$	$= \inf_{y\in Y} \|x-y\|$, distance between x and Y
$\mathfrak{D}(.)$	... domain of an operator
e	... exponential function, $\mathrm{e}^z = \exp(z)$
$\mathbb{E}(A)$	... expectation of an operator A, 55
$\mathcal{F}$	... Fourier transform, 161
H	... Schrödinger operator, 221
H_0	... free Schrödinger operator, 167
$H^m(a,b)$	... Sobolev space, 85
$H^m(\mathbb{R}^n)$	... Sobolev space, 164
hull(.)	... convex hull
$\mathfrak{H}$	... a separable Hilbert space
i	... complex unity, $\mathrm{i}^2 = -1$
$\mathbb{I}$	... identity operator
Im(.)	... imaginary part of a complex number
inf	... infimum
$\mathrm{Ker}(A)$	... kernel of an operator A, 22

$\mathfrak{L}(X,Y)$	... set of all bounded linear operators from X to Y, 23
$\mathfrak{L}(X)$	$= \mathfrak{L}(X,X)$
$L^p(X,d\mu)$	... Lebesgue space of p integrable functions, 26
$L^p_{loc}(X,d\mu)$	... locally p integrable functions, 31
$L^p_c(X,d\mu)$	... compactly supported p integrable functions
$L^\infty(X,d\mu)$	... Lebesgue space of bounded functions, 26
$L^\infty_\infty(\mathbb{R}^n)$	... Lebesgue space of bounded functions vanishing at ∞
$\ell^1(\mathbb{N})$	... Banach space of summable sequences, 13
$\ell^2(\mathbb{N})$	... Hilbert space of square summable sequences, 17
$\ell^\infty(\mathbb{N})$	... Banach space of bounded summable sequences, 13
λ	... a real number
$m_a(z)$	... Weyl m-function, 199
$M(z)$	... Weyl M-matrix, 211
max	... maximum
$\mathcal{M}$	... Mellin transform, 251
μ_ψ	... spectral measure, 95
$\mathbb{N}$	... the set of positive integers
$\mathbb{N}_0$	$= \mathbb{N} \cup \{0\}$
$o(x)$	... Landau symbol little-o
$O(x)$	... Landau symbol big-O
Ω	... a Borel set
$\Omega_\pm$	... wave operators, 247
$P_A(.)$	... family of spectral projections of an operator A, 96
$P_\pm$	... projector onto outgoing/incoming states, 250
$\mathbb{Q}$	... the set of rational numbers
$\mathfrak{Q}(.)$	... form domain of an operator, 97
$R(I,X)$	... set of regulated functions, 112
$R_A(z)$	... resolvent of A, 74
$\mathrm{Ran}(A)$	... range of an operator A, 22
$\mathrm{rank}(A)$	$= \dim \mathrm{Ran}(A)$, rank of an operator A, 127
$\mathrm{Re}(.)$	... real part of a complex number
$\rho(A)$	... resolvent set of A, 73
$\mathbb{R}$	... the set of real numbers
$S(I,X)$	... set of simple functions, 112
$\mathcal{S}(\mathbb{R}^n)$	... set of smooth functions with rapid decay, 161
$\mathrm{sign}(x)$	... $+1$ for $x > 0$ and -1 for $x < 0$; sign function
$\sigma(A)$	... spectrum of an operator A, 73
$\sigma_{ac}(A)$	... absolutely continuous spectrum of A, 106
$\sigma_{sc}(A)$	... singular continuous spectrum of A, 106
$\sigma_{pp}(A)$	... pure point spectrum of A, 106
$\sigma_p(A)$	... point spectrum (set of eigenvalues) of A, 103
$\sigma_d(A)$	... discrete spectrum of A, 145
$\sigma_{ess}(A)$	... essential spectrum of A, 145

span(M)	...set of finite linear combinations from M, 14
sup	...supremum
supp(f)	...support of a function f, 7
$\mathbb{Z}$	...the set of integers
z	...a complex number

$\sqrt{z}$	...square root of z with branch cut along $(-\infty, 0]$
z^*	...complex conjugation
A^*	...adjoint of A, 59
$\overline{A}$	...closure of A, 63
$\hat{f}$	$= \mathcal{F}f$, Fourier transform of f, 161
$\check{f}$	$= \mathcal{F}^{-1}f$, inverse Fourier transform of f, 163
$\|.\|$	...norm in the Hilbert space $\mathfrak{H}$, 17
$\|.\|_p$	...norm in the Banach space L^p, 25
$\langle ., .. \rangle$	...scalar product in $\mathfrak{H}$, 17
$\mathbb{E}_\psi(A)$	$= \langle \psi, A\psi \rangle$, expectation value, 56
$\Delta_\psi(A)$	$= \mathbb{E}_\psi(A^2) - \mathbb{E}_\psi(A)^2$, variance, 56
Δ	...Laplace operator, 167
∂	...gradient, 162
∂_α	...derivative, 161
$\oplus$	...orthogonal sum of linear spaces or operators, 45, 79
$M^\perp$	...orthogonal complement, 43
A'	...complement of a set
(λ_1, λ_2)	$= \{\lambda \in \mathbb{R} \,\vert\, \lambda_1 < \lambda < \lambda_2\}$, open interval
$[\lambda_1, \lambda_2]$	$= \{\lambda \in \mathbb{R} \,\vert\, \lambda_1 \le \lambda \le \lambda_2\}$, closed interval
$\psi_n \to \psi$	...norm convergence, 12
$\psi_n \rightharpoonup \psi$	...weak convergence, 49
$A_n \to A$	...norm convergence
$A_n \xrightarrow{s} A$	...strong convergence, 50
$A_n \rightharpoonup A$	...weak convergence, 50
$A_n \xrightarrow{nr} A$	...norm resolvent convergence, 153
$A_n \xrightarrow{sr} A$	...strong resolvent convergence, 153

Index

Quantum mechanics and the theory of operators on Hilbert space have been deeply linked since their beginnings in the early twentieth century. States of a quantum system correspond to certain elements of the configuration space and observables correspond to certain operators on the space. This book is a brief, but self-contained, introduction to the mathematical methods of quantum mechanics, with a view towards applications to Schrödinger operators.

Part 1 of the book is a concise introduction to the spectral theory of unbounded operators. Only those topics that will be needed for later applications are covered. The spectral theorem is a central topic in this approach and is introduced at an early stage. Part 2 starts with the free Schrödinger equation and computes the free resolvent and time evolution. Position, momentum, and angular momentum are discussed via algebraic methods. Various mathematical methods are developed, which are then used to compute the spectrum of the hydrogen atom. Further topics include the nondegeneracy of the ground state, spectra of atoms, and scattering theory.

This book serves as a self-contained introduction to spectral theory of unbounded operators in Hilbert space with full proofs and minimal prerequisites: Only a solid knowledge of advanced calculus and a one-semester introduction to complex analysis are required. In particular, no functional analysis and no Lebesgue integration theory are assumed. It develops the mathematical tools necessary to prove some key results in nonrelativistic quantum mechanics.

Mathematical Methods in Quantum Mechanics is intended for beginning graduate students in both mathematics and physics and provides a solid foundation for reading more advanced books and current research literature. It is well suited for self-study and includes numerous exercises (many with hints).

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