

# Preface

The spectral theory of linear operators in Hilbert spaces is the most important tool in the mathematical formulation of quantum mechanics; in fact, linear operators and quantum mechanics have had a symbiotic relationship. However, typical physics textbooks on quantum mechanics give just a rough sketch of operator theory, occasionally treating linear operators as matrices in finite-dimensional spaces; the implicit justification is that the details of the theory of unbounded operators are involved and those texts are most interested in applications. Further, it is also assumed that mathematical intricacies do not show up in the models to be discussed or are skipped by “heuristic arguments.” In many occasions some questions, such as the very definition of the hamiltonian domain, are not touched, leaving an open door for controversies, ambiguities and choices guided by personal tastes and ad hoc prescriptions. All in all, sometimes a blank is left in the mathematical background of people interested in nonrelativistic quantum mechanics.

Quantum mechanics was the most profound revolution in physics; it is not natural to our common sense (check, for instance, the wave-particle duality) and the mathematics may become crucial when intuition fails. Even some very simple systems present nontrivial questions whose answers need a mathematical approach. For example, the Hamiltonian of a quantum particle confined to a box involves a choice of boundary conditions at the box ends; since different choices imply different physical models, students should be aware of the basic difficulties intrinsic to this (in principle) very simple model, as well as in more sophisticated situations. The theory of linear operators and their spectra constitute a wide field and it is expected that the selection of topics in this book will help to fill this theoretical gap. Of course this selection is greatly biased toward the preferences of the author.

Besides the customary role of working as a computational instrument, a mathematically rigorous approach could lead to a more profound insight into the nature of quantum mechanics, and provide students and researchers with appropriate tools for a better understanding of their own research work. So the first aim of this book is to present the basic mathematics of nonrelativistic quantum mechanics of one particle, that is, developing the spectral theory of self-adjoint operators in infinite-dimensional Hilbert spaces from the beginning. The reader is assumed to have had some contact with functional analysis and, in applications to differ-

ential operators, with rudiments of distribution theory. Traditional results of the theory of linear operators in Banach spaces are addressed in Chapter 1, whereas necessary results of Sobolev spaces are described in Chapter 3. The definition and basic properties of (unbounded) self-adjoint operators appear in Chapter 2.

The second aim of this book is to give an overview of many of the basic functional analysis aspects of quantum theory, from its physical principles to the mathematical methods. This end is illustrated by:

1. The use of von Neumann theory of self-adjoint extensions (2), Fourier transform (3), sesquilinear forms (4), Kato-Rellich and KLMN theorems (6) and boundary triples (7) as tools to properly define Schrödinger (self-adjoint) operators in quantum mechanics. These matters are developed in the chapters indicated above in parentheses.
2. The spectral theorem and first applications in Chapters 8 and 9.
3. Convergence of (unbounded) self-adjoint operators in Chapter 10.
4. Spectral decomposition (essential, discrete, continuous and point) in Chapters 11 and 12.

In case of time evolution, which is ruled by the quantum energy operator, item 1 above is closely related to the question in classical mechanics whether the motion is unambiguously determined by the force.

Another aim of this book is to strive to present many examples illustrating concepts and build up confidence with methods. Some examples are simple and are meant to reduce the effort of beginning graduate students to learn the subject of spectral theory and its relation to quantum mechanics.

The last aim of the book is to discuss the relation between spectral type of the hamiltonian (energy) operator and asymptotic quantum dynamics, i.e., the quantum behavior as time goes to infinity. In Chapter 5, the existence of quantum dynamics is shown to be equivalent to the self-adjointness of the Hamiltonian, but the discussion is not restricted to time evolution and the general theory of unitary evolution groups is addressed in detail. Various aspects of the role played by the spectral type in quantum dynamics are given in Chapter 13. Some results seem not to have appeared in book form yet, such as the discussions on precompact orbits and almost periodic trajectories. Chapters 11, 12 and 13 make heavy use of spectral measures and are more advanced than previous chapters.

Selected quantum relations are discussed in Chapter 14. The idea is to complement a text that emphasizes mathematics with additional rigorous approaches to some standard quantum concepts; e.g., why the quantum observables are represented by self-adjoint operators instead of just hermitian ones. But no exhaustive presentation of quantum relations should be expected and parallel reading of traditional books on quantum mechanics is highly recommended.

The book does not offer a quantum mechanics course, but the necessary quantum concepts are introduced when needed (usually with Planck's constant

$\hbar = 1$  and mass particle  $m = 1/2$ ). Hence, it can also be useful to readers who are only interested in an introduction to spectral theory, since its focus is mathematics and proofs of theorems. The level is suitable for graduate students (or advanced undergraduates) who already have some familiarity with linear functional analysis. Thus, more advanced methods in spectral theory, mainly those related to singular continuous and dense point spectra, are not discussed (see [DeKr05] for a collection of advanced methods and the four volumes by Reed and Simon in the references); this is the reason for the term “Intermediate” in the title of the book. However, a certain level of mathematical literacy is desired from the reader.

Different readers may have different backgrounds, and each one will easily find which sections to skip and a suitable pathway to the particular topics of interest. But most of them will usually start on the introduction of a spectrum in Section 1.5 or Chapter 2. After working through this book, a student should be able to follow more specialized texts and research articles, and should find it easier to select a topic for future research.

Exercises present different levels of difficulties; many of them are related to missing details in proofs and examples. Due to the nature of the book, the set of references includes literature on both physics and mathematics.

Parts of the book have been used in courses addressed to graduate students interested in spectral theory at the Department of Mathematics of the Federal University of São Carlos, in 2004 and 2006; in fact, the book grew out of such lectures. The author thanks students and colleagues who have attended those courses and made helpful comments. Partial financial support by a Brazilian federal agency, CNPq, is very much acknowledged.

I want to thank the patience and support of my wife, Ana Teresa, and our children, Daniel and Natália, that gave me stability during the revisions of the text.

Hopefully, you, mathematician or physicist, will enjoy reading the book and will profit from it. The following page on the internet

<http://www.dm.ufscar.br/~oliveira/ISTbook.html>

is related to this book and it may include a possible errata page. Any remark, suggestion and correction (including those that have arisen from “copy-paste” manipulations) from readers will be welcome!

May 2008

São Carlos,  
*César R. de Oliveira*

Intermediate Spectral Theory and Quantum Dynamics

de Oliveira, C.R.

2009, XIII, 410 p., Hardcover

ISBN: 978-3-7643-8794-5

A product of Birkhäuser Basel