NON-HERMITIAN QUANTUM MECHANICS

Non-Hermitian quantum mechanics (NHQM) is an important alternative to the standard (Hermitian) formalism of quantum mechanics, enabling the solution of otherwise difficult problems. The first book to present this theory, it is useful to advanced undergraduate and graduate students and researchers in physics, chemistry and engineering.

NHQM provides powerful numerical and analytical tools for the study of resonance phenomena – perhaps one of the most striking events in nature. It is especially useful for problems whose solutions cause extreme difficulties within the structure of a conventional Hermitian framework. NHQM has applications in a variety of fields, including optics, where the refractive index is complex; quantum field theory, where the parity-time (PT) symmetry properties of the Hamiltonian are investigated; and atomic and molecular physics and electrical engineering, where complex potentials are introduced to simplify numerical calculations.

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Cambridge University Press
978-0-521-88972-8 - Non-Hermitian Quantum Mechanics
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CAMBRIDGE
UNIVERSITY PRESS

CAMBRIDGE UNIVERSITY PRESS
Cambridge, New York, Melbourne, Madrid, Cape Town, Singapore,
São Paulo, Delhi, Dubai, Tokyo, Mexico City

Cambridge University Press
The Edinburgh Building, Cambridge CB2 8RU, UK

Published in the United States of America by Cambridge University Press, New York

www.cambridge.org
Information on this title: www.cambridge.org/9780521889728

First published 2011

Printed in the United Kingdom at the University Press, Cambridge

A catalogue record for this publication is available from the British Library

Library of Congress Cataloguing in Publication data
Moiseyev, Nimrod, 1947–
Non-Hermitian quantum mechanics / Nimrod Moiseyev.
p. cm.
Includes bibliographical references and index.
ISBN 978-0-521-88972-8 (hardback)
1. Quantum theory – Mathematics. 2. Hermitian structures. 3. Resonance.
4. Hermitian symmetric spaces. I. Title.
QC174.17.M35M65 2011
530.12 – dc22 2010040292

ISBN 978-0-521-88972-8 Hardback

To the memory of my parents Rachel and Itzhak
who taught me to wonder

The Lively Imagination/Zelda

For the lively imagination
Holds a secret key,
Granted to the ignorant and unlettered,
That unlocks the ivory doors of science.
It enters the soaring towers,
Ambles through the equation-teeming dark –
And whistles there in wonder
Like an unruly youth.

Translated from the Hebrew by *Amitai Halevi*

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Preface

This is the first book ever written that presents non-Hermitian quantum mechanics (NHQM) as an alternative to the standard (Hermitian) formalism of quantum mechanics. Previous knowledge of the basic principles of quantum mechanics and its standard formalism is required.

The standard formalism is based on the requirement that all observable properties of a dynamic nature are associated with the real eigenvalues of a special class of operators, called Hermitian operators. All textbooks use Hermitian Hamiltonians in order to ensure conservation of the number of particles. See, for example, the monumental book of Dirac on *The Principles of Quantum Mechanics*.

The motivation for the derivation of the NHQM formalism is twofold.

The first is to be able to address questions that can be answered **only** within this formalism. For example:

- in optics, where complex index of refraction are used;
- in quantum field theory, where the parity–time (PT) symmetry properties of the Hamiltonian are investigated;
- in cases where the language of quantum mechanics is used, even though the problems being addressed are within classical statistical mechanics or diffusion in biological systems;
- in cases where complex potentials are introduced far away from the interaction region of the particles. This approach simplifies the numerical calculations and avoids artificial interference effects caused by reflection of the propagated wave packets from the edge of the grid.

The second is the desire to tackle problems that can, in principle, also be solved within the conventional Hermitian framework, but only with extreme difficulty, whereas the NHQM formalism enables a much simpler and more elegant solution. Moreover it provides the insight that is required in order to predict novel physical phenomena and to design the corresponding experiments. It is most useful in exploration of the **resonance** phenomena, where particles are temporarily trapped by the potential.

In their book on non-relativistic quantum mechanics, Landau and Lifshitz wrote about the need for NHQM:

> Until now we have always considered solutions of the Schrödinger equation with a boundary condition requiring the finiteness of the wavefunction at infinity. Instead of this, we shall look for solutions which represent an outgoing spherical wave at infinity; this corresponds to the particle finally leaving the system when it disintegrates. Since such a boundary condition is complex, we cannot assert that the eigenvalues of the energy must be real. (Section 132 on Resonance at a quasi-discrete level).

The resonance phenomena are some of the most striking phenomena in nature. Resonances are associated with metastable states of a system that has sufficient energy to break up into two or more subsystems. These systems can be nuclei, atoms, molecules, solids, nano-structured materials and condensates. The subsystems may contain elementary particles and/or neutral or negatively/positively charged atomic or molecular ions. The systems whose dynamics is controlled by the resonance phenomena can be as small as protonium (the exotic atom consisting of a proton and an anti-proton) or a helium atom, or as large as a protein.

However, because of the exponential divergence of the asymptotes of the resonance solutions, the derivation of the NHQM formalism became possible **only** after the derivation of the complex scaling transformation by Balslev-Combes and by Barry Simon, with which resonance wavefunctions become square integrable as **bound states** in the standard formalism. The non-Hermitian formalism avoids the need to carry out complicated wave-packet-propagation calculations in order to describe resonance phenomena, and enables the association of a given resonance phenomenon as it appears in an atomic, molecular, nuclear or chemical system with a **single** square-integrable eigenfunction of the complex-scaling Hamiltonian. Therefore, the non-Hermitian formalism, based on this kind of transformation, enables the calculation of cross sections and dynamical properties of systems controlled by their resonance states, by using computational algorithms that were originally developed for bound states in conventional Hermitian quantum mechanics.

Nevertheless, many questions remain unanswered. For example: what is the solution of the time-asymmetric problem in non-Hermitian quantum mechanics? It arises because the time-dependent phase factor, $\exp(-\mathrm{i}Et/\hbar)$, which since $-2\mathrm{Im}(E)$, the decay rate, is necessarily positive, diverges exponentially as $t \to -\infty$. What are the implications and physical manifestations of the incomplete spectrum of a non-Hermitian Hamiltonian that is obtained when two or more eigenstates coalesce to a single self-orthogonal state? What is the physical interpretation of the phase of the complex probability density in non-Hermitian quantum mechanics and how would time-dependent expectations of measurable quantities be calculated?

The answers to these questions that are given in this book are based mainly on my research over the last three decades. It began with my work in Madison, Wisconsin with Phil Certain and Frank Weinhold on the properties of the complex-scaled non-Hermitian Hamiltonian, and then through many years of research with my PhD students and post-doctoral fellows and with my colleagues as well. (I am fortunate to have been surrounded by so many gifted people for such a long period of time.) Thirty years ago, in collaboration with the mathematician Shmuel Friedland, we found that self-orthogonality, the coalescence of two or more eigenstates, is related to the incomplete spectrum of the non-Hermitian complex-scaled Hamiltonian. However, it was not until my most recent series of studies that it was shown to be an observable phenomenon that may have different effects in different fields of physical science.

Aside from presenting the non-Hermitian formalism of quantum mechanics, the purpose of this textbook is to provide many solved problems that will provide a better understanding of the foundations of quantum mechanics, to explain the algorithms for calculating the resonance measurable quantities, and to illustrate the applications of the formalism to physics, chemistry and technology. It should be noted that many of the exercises are not included for honing the skills of the reader, but rather for introducing him/her to additional details of the theory – which can be skipped by readers who may not be interested or conversant with the more technical details.

This textbook is designed for use by graduate and undergraduate students that have already attended a basic course in quantum mechanics. However, for the sake of coherence and in order to make the book more self-contained, the exercises also include problems and solutions for Hermitian cases.

I am grateful to many of my students and colleagues, without whom I would not have been able to do the scientific work that laid the groundwork for this book. Above all, I wish to express my thanks to my student Dr Ido Gilary, who has carefully read the manuscript and checked the solutions given in the book, and whose cogent comments have helped me present the theory more coherently and avoid many pitfalls. Any errors or inaccuracies that remain in the final version are my responsibility alone.

Last but by no means least, I thank my wife Etty, my children Gilead and Hamutal, my daughter and son-in-law Vardit and David, and my grandchildren Noam and Jonathan for their patience, care and love, that gave me the peace of mind needed to do science with joy and fun.