Nonrelativistic Quantum Mechanics

Anton Z. Capri

Nonrelativistic Quantum Mechanics

Anton Z. Capri
Physics Department, University of Alberta
Edmonton, Alberta, Canada

To Kim, Karin, Irene and Skaidrite for giving me time and love.

Sponsoring Editor: Richard W. Mixter Production Editor: Karen Gulliver

Copyright © 1985 by The Benjamin/Cummings Publishing Company, Inc.

All rights reserved. No part of this publication may be reproduced, stored in a retrieval system, or transmitted, in any form or by any means, electronic, mechanical, photocopying, recording, or otherwise, without the prior written permission of the publisher. Printed in the United States of America. Published simultaneously in Canada.

Library of Congress Cataloging in Publication Data

Capri, Anton Z.
 Non relativistic quantum mechanics.

Includes index.

1. Quantum theory. 2. Perturbation (Quantum dynamics)

I. Title.

QC174.12.C35 1985 ISBN 0-8053-1505-\$ 530.1'2

85-14933

ABCDEFGHIJ-MA-898765



The Benjamin Cummings Publishing Company, Inc. 2727 Sand Hill Road
Menlo Park, California 94025

Editor's Foreward

Everyone concerned with the teaching of physics at the advanced undergraduate or graduate level is aware of the continuing need for a modernization and reorganization of the basic course material. Despite the existence today of many good textbooks in these areas, there is always an appreciable time-lag in the incorporation of new viewpoints and techniques which result from the most recent developments in physics research. Typically these changes in concepts and material take place first in the personal lecture notes of some of those who teach graduate courses. Eventually, printed notes may appear, and some fraction of such notes evolve into textbooks or monographs. But much of this fresh material remains available only to a very limited audience, to the detriment of all. This series aims at filling this gap in the literature of physics by presenting occasional volumes with a contemporary approach to the classical topics of physics at the advanced undergraduate and graduate level. Clarity and soundness of treatment will, we hope, mark these volumes, as well as the freshness of the approach.

Another area in which the series hopes to make a contribution is by presenting useful supplementing material of well-defined scope. This

Editor's Foreward

may take the form of a survey of relevant mathematical principles, or a collection of reprints of basic papers in a field. Here the aim is to provide the instructor with added flexibility through the use of supplements at relatively low cost.

The scope of both the lecture notes and supplements is somewhat different from the "Frontiers in Physics" series. In spite of wide variations from institution to institution as to what comprises the basic graduate course program, there is a widely accepted group of "bread and butter" courses that deal with the classic topics in physics. These include: Mathematical methods of physics, electromagnetic theory, advanced dynamics, quantum mechanics, statistical mechanics, and frequently nuclear physics and/or solid-state physics. It is chiefly these areas that will be covered by the present series. The listing is perhaps best described as including all advanced undergraduate and graduate courses which are at a level below seminar courses dealing entirely with current research topics.

Finally, because the series represents a continuing experiment on the part of the editors and the publisher, suggestions from interested readers as to format, contributors, and contributions will be most welcome.

DAVID PINES

Preface

Most textbooks start as a set of lecture notes which expand and undergo numerous revisions over the years. The present version is no exception and is the culmination of many revisions of such lecture notes. I have taught quantum mechanics at several different levels and thus attempted to make this book of sufficiently broad scope for different courses. The book includes material for undergraduate courses as well as a one-semester graduate course. As a guide for possible division of the material in this book I have included a few pages in the following section entitled "How to use this Book".

It is a long way from lecture notes to a text-book and on this journey I have been greatly helped by many people. My first debt is to my students who forced me to clarify and expand my lecture notes. Without their prodding this book would never have been started.

Dr. M. Razavy has also been most generous with his time and ideas. Not only did he test this book in his quantum mechanics classes, but he willingly proof-read all the present version. He also helped with many pertinent references and comments; his criticism of chapter 21 was particularly useful. Without his constant encouragement and support my enthusiasm would have flagged many times and this book might never have been written.

Preface

During the early stages, Dr. W. Brouwer also helped considerably with his detailed criticisms of the first fourteen chapters. I thank him for his generous contribution of time and ideas.

The first version of this book was expertly typed by Mrs. M. Yiu. Had she not been here to read my scrawl, I am sure this book would never been written. I thank her for her patience and tolerance.

The diagrams are due to the heroic efforts of Mrs. J. Hube. Her attention to detail turned some rather skimpy sketches into actual diagrams. I am most grateful for her skills.

Finally, I acknowledge with many thanks the expertly accomplished job of preparing the final manuscript. This was ably handled by Christine Fischer and Laura Heiland. Their friendly attitude did much to make a painful job easier.

I would also like to thank all of my colleagues who, in one way or another, influenced me during our coffee-room discussions. Their contributions, although less tangible, are nevertheless very real.

It is my hope that in writing this book I may have helped a few students to discover the beauty of quantum mechanics.

Anton Z. Capri

Edmonton, Alberta April, 1985 How to Use This Book

This book is designed for use in any of the following programs:

- A) A one-semester introductory course for undergraduates;
- B) A two-semester introductory course for undergraduates;
- .C) A one-semester graduate courses.

To indicate which material is suitable for inclusion in any of the above programs I have added the appropriate letter or letters "A,B,C" after the title in the Table of Contents. Thus, for example, all section headings for Chapter 1, except 1.10 and 1.11, are followed by the letters "AB" to indicate that this material is suitable for both a one-semester introductory course as well as a two-semester course. Sections 1.10 and 1.11 are labelled only B and should be omitted in a one-semester undergraduate course.

The material to be included will also vary from class to class. Thus it is not feasible, nor should it be attempted, to include all the sections marked with a "B" in a two-semester undergraduate course. For example, I have found that I could include either the Rayleight-Ritz variational approach or a somewhat watered-down version of the WKB approximation in a two-semester undergraduate course, but not both.

How to Use This Book

Similarly in a one-semester graduate course a selection from the material marked "C" is necessary. This will, of course, depend on the special interests of the students. The point is that not all the material in any given course division (A,B or C) can be covered in the time normally allotted for such a course. The interests of classes vary from year to year and so I have included extra topics from which a selection can be made.

•	tue presedong of Classical wecusules	1
1.1	Blackbody Radiation (AB)	2
1.2	Stability of Atoms - Discrete Spectral Lines (AB)	6
1.3	Photoelectric Effect (AB)	10
1.4	Wave Particle Duality (AB)	12
1.4.1	Reflection	13
1.4.2	Refraction	13
1.5	De Broglie's Hypothesis (AB)	14
1.6	The Compton Effect (AB)	15
1.7	The Davisson-Germer Experiment (AB)	18
1.8	The Franck-Hertz Effect (AB)	21.
1.9	Planck's Radiation Law (AB)	23
1.10	Einstein's Model for Specific Heat (B)	24
1.11	Bohr Theory and the Hydrogen Atom (B)	28
2	Review of Classical Mechanics	34
2.1	Classical Mechanics of a Particle in One Dimension (AB)	34
2.2	Lagrangian and Hamiltonian Formulation (B)	41
2.3	Contact Transformations and Hamilton-Jacobi Theory (B)	44
2.4	Interpretation of the Action-Angle Variable (B)	52

2.5	Hydrogen Atom for Bohr-Sommerfeld Quantization (B)	54
2.6	The Schrödinger Equation (B)	59
3	Planatary Sustan	65
	Elementary Systems	65
3.1	Plane Wave Solutions (AB)	66
3.2	Conservation Law for Particles (AB)	67
3.3	Young's Double Slit Experiment (A)	69
3.4	The Superposition Principle and Group Velocity (AB)	70
3.5	Formal Considerations (AB)	74
3.6	Ambiguities (AB)	76
3.6.1	Use of Different Coordinate Systems	77
3.6.2	Noncommunatuity	78
3.7	Interaction with an Electromagnetic Field (B)	80
4	One-Dimensional Problems	85
4.1	Introduction (AB)	85
4.2	Finite Square Well - Bound States (AB)	87
4.3	Parity (AB)	91
4.4	Scattering from a Step-Function Potential (AB)	95
4.5	Infinite Square Well - Particle in a Box (AB)	110
4.6	Time Reversal (B)	111
5	More One Dimensional Problems	116
5.1	General Considerations (AB)	116
5.2	Tunneling Through a Square Barrier (AB)	121
5.3	The Simple Harmonic Oscillator (AB)	125
5.4	The Delta Function (AB)	131
5.5	Attractive Delta Function Potential (AB)	134
5.6	Repulsive Delta Function Potential (AB)	136
5.7	Finite Square Well - Scattering and Phase Shifts (B)	138
	Time square werr season, and amore and the	:
6	Mathematical Foundations of Quantum Mechanics	145
6.1	Geometry of Hilbert Space (AB)	145
6.2	L ₂ - A Model Hilbert Space (AB)	150

6.3	Operators on Hilbert Space - Mainly Definitions (BC)	153
6.4	The Cayley Transform and Self-Adjoint Operators (BC)	161
6.5	Some Properties of Self-Adjoint Operators (AB)	166
6.6	Classification of Symmetric Operators (BC)	170
6.7	Spontaneously Broken Symmetry (BC)	179
7	Physical Interpretation of Quantum Mechanics	187
7.1	Assumption (A1) - Physical States (ABC)	187
7.2	Assumption (A2) - Observables (ABC)	188
7.3	Assumption (A3) - Probabilities (ABC)	189
7.4	Assumption (A4) - Reduction of the Wave Packet (ABC)	194
7.5	Example (AB)	195
7.6	Compatibility Theorem and Uncertainty Principle (ABC)	197
7.7	The Heisenberg Microscrope (ABC)	199
7.8	Assumption (A5) - The Schrödinger Equation (ABC)	203
7.9	Time Evolution of Expectation Values and	
	Constants of the Motion (BC)	205
7.10	Time-Energy Uncertainty Relation (BC)	206
7.11	Time Evolution of Probability Amplitudes (BC)	210
8	Distributions, Fourier Transforms, and Rigged Hilbert Spaces	219
8.1	Functionals (BC)	219
8.2	Fourier Transforms (BC)	227
8.3	Rigged Hilbert Space (BC)	229
9	Algebraic Approach to Time-Independent Problems	236
9.1	Simple Harmonic Oscillator (AB)	236
9.1.1	Expectation Values	244
9.2	The Rigid Rotator (ABC)	247
9.3	Rigid Rotator in Three Dimensions - Angular Momentum (BC)	254
9.4	Algebraic Approach to Angular Momentum (BC)	257
9.5	Rotations and Rotational Invariance (BC)	257
9.6	Spin Angular Momentum (BC)	272

10	Central Force Problems	281
10.1	The Radial Equation (ABC)	282
10.2	Infinite Square Well (ABC)	286
10.3	Simple Harmonic Oscillator: Separation in	
	Cartesian Coordinates (ABC)	289
10.3.	1 Degeneracy	291
10.4	Simple Harmonic Oscillator: Separation in	271
	Spherical Coordinates (BC)	292
10.5	The Hydrogenic Atom (ABC)	296
10.6	Reduction of the Two-Body Problem (BC)	306
11	Transformation Theory	311
11.1	Rotations in a Vector Space (BC)	312
11.2	Example 1 - Fourier Transform of Hermite Functions (BC)	315
11.3	Dirac Notation (BC)	316
11.4	Example 2 - Angular Momentum (BC)	323
11.5	The Schrödinger Picture (BC)	327
11.6	Reisenberg Picture (BC)	328
11.7	Dirac or Interaction Picture (C)	333
12	Time-Independent Non-Degenerate Perturbation Theory	339
12.1	Rayleigh-Schrödinger Perturbation Theory for	
*	Stationary States (BC)	340
12.2	First Order Perturbations (BC)	343
12.3	Example 1 - Anharmonic Oscillator (BC)	345
12.4	Example 2 - Ground State of Helium-like Ions (BC)	346
12.5	Second Order Perturbations (BC)	349
12.6	Example 3 - Displaced Simple Harmonic Oscillator (BC)	350
12.7	Non-degenerate Perturbations to All Orders (C)	353
12.8	Sum Rule for Second Order Perturbation Theory (BC)	357
12.9	Linear Stark Effect (BC)	361

13	Time-Independent Degenerate Perturbation Theory	367
13.1	Two Levels: Rayleigh-Schrödinger Method for	
	Degenerate Levels (BC)	368
13.2	General Rayleigh-Schrödinger Method for	
•	Degenerate Levels	372
13.3	Example: Spin Hamiltonian (BC)	374
13.3.1	Exact Solution	375
13.3.2	Rayleigh - Schrödinger Solution	377
14	Further Approximation Methods	381
14.1	Rayleigh-Ritz Method (BC)	383
14.2	Example 1 - Simple Harmonic Oscillator (BC)	386
14.3	Example 2 - He Ground State (BC)	387
14.4	The W.K.B. Approximation (BC)	389
14.4.1	Turning Points	395
14.5	Example 3 - W.K.B. Applied to a Potential Well (BC)	401
14.6	Special Boundaries (BC)	404
14.7	Example 4 - W.K.B. Approximation for Tunneling (BC)	405
15	Time-Dependent Perturbation Theory	411
15.1	Formal Considerations (C)	411
15.2	Direct Computations of Transition Amplitudes (BC)	416
15.3	Periodic Perturbation of Finite Duration (BC)	418
15.4	Photo-Ionization of Hydrogen Atom (BC)	422
15.5	The Adiabatic Approximation (BC)	427
15.6	The Sudden Approximation (BC)	433
15.7	Dipole in a Time-Dependent Magnetic Field (BC)	435
15.7.1	Oscillatory Perturbation	437
15.7.2	Slowly Varying Perturbation	439
15.7.3	Sudden Approximation	441
16	Applications	447
16.1	Gauge Transformations (C)	447

16.2	Motion in a Uniform Magnetic Field - Landau Levels (C)	452
16.3	The Quantum Hall Effect (C)	454
16.4	Motion in s Uniform Magnetic Field	
	- Heisenberg Equations (C)	457
16.5	Spin and Spin-Orbit Coupling (C)	469
16.6	Alkali Spectra (C)	471
16.7	Addition of Angular Momenta (C)	474
16.8	Example 1 - Two Spin 1/2 States (C)	479
16.9	Example 2 - Spin 1/2 and Orbital Angular Momentum (C)	480
16.10	The Weak-Field Zeeman Effect (C)	481
17	Scattering Theory: Time Dependent Formulation	488
17.1	Classical Scattering Theory (BC)	489
17.2	Asymptotic States in the Schrödinger Picture (C)	491
17.3	The Moller Wave Operators (C)	493
17.4	Green's Functions and Propagators (C)	496
17.5	Integral Equations for the Propagators:	
,	Asymptotic States (C)	500
17.6	Cross-sections (BC)	502
17.7	The Lippmann-Schwinger Equations (C)	503
17.8	The S-Matrix and the Scattering Amplitude (C)	506
18	Scattering Theory: Time Independent Formulation	513
18.1	The Scattering Amplitude (BC)	513
18.2	Green's Functions and The Lippmann-Schwinger Equations (C)	516
18.3	The Born Approximation (BC)	521
18.4	Example - The Yukawa Potential (BC)	524
18.5	The Free Schrödinger Equation in Spherical Coordinates (BC)	526
18.6	Partial Wave Analysis (BC)	534
18.7	Phase Shifts (BC)	537
18.8	The Optical Theorem - Unitarity Bound (BC)	539
19	Further Topics in Potential Scattering	544
19.1	Example - The Square Well (BC)	545

644

100		
19.2	Partial Wave Analysis of the	
	Lippmann-Schwinger Equation (C)	549
19.3	Effective Range Approximation (C)	551
19.4	The Glauber or Eikonal Approximation (C)	557
•		
20	Systems of Identical Particles	569
20.1	Two Identical Particles (BC)	570
20.2	The Hydrogen Molecule (BC)	572
20.3	N Identical Particles (C)	579
20.4	Non-Interacting Fermions (C)	582
20.5	Non-Interacting Bosons (C)	584
20.6	Occupation Number Space and Second Quantization for	
	Bosons (C)	586
20.7	Occupation Number Space and Second Quantization for	-
•	Fermions (C)	589
20.8	Field Operators (C)	593
20.9	Representation of Operators (C)	. 597
20.10	Heisenberg Picture (C)	601
21	Quantum Statistical Mechanics	608
21.1	Introduction (C)	608
21.2	The Density matrix (C)	610
21.2.1	The Microcanonical Ensemble.	610
21.2.2	The Canonical Ensemble	612
21.2.3	Grand Canonical Ensemble	613
21.3	The Ideal Gases (C)	610
21.4	General Properties of the Density Matrix (C)	623
21.5	The Density Matrix and Polarization (C)	626
21.6	Composite Systems (C)	630
21.7	The Quantum Theory of Measurement (C)	634
21.8	Conclusion (C)	639

Index

Chapter 1

The Breakdown of Classical Mechanics

During the nineteenth century many of the great advances in physics of the eighteenth century were consolidated and extended. In addition, the theory of electromagnetism was completed by J.C. Maxwell. Except for a few unexplained effects or anomalies there seemed little more in terms of fundamental physics to be done by the beginning of the twentieth century. Yet it is precisely in the year 1900 that quantum theory starts with Planck's formula for blackbody radiation.

Soon there were a host of experimental results, both new ones and earlier ones that again attracted attention. All of these pointed to flaws in the physics of the nineteenth century. In almost all cases these anomalies resulted when Newtonian mechanics and electromagnetism were simultaneously involved. In trying to elucidate these various experimental facts a new theory of physics, quantum theory, was born.

In the next few sections we briefly examine several of these experiments and discuss them with some modern hindsight. First we consider blackbody radiation from the prequantum or classical point of view. We then turn to a consideration of the stability of the classical Rutherford atom. Although Rutherford had experimentally demonstrated the planetlike structure of the electrons in atoms, his model caused a lot of theoretical problems.