Applied Quantum Mechanics, Second Edition

Electrical and mechanical engineers, materials scientists and applied physicists will find Levi's uniquely practical explanation of quantum mechanics invaluable. This updated and expanded edition of the bestselling original text now covers quantization of angular momentum and quantum communication, and problems and additional references are included. Using real-world engineering examples to engage the reader, the author makes quantum mechanics accessible and relevant to the engineering student. Numerous illustrations, exercises, worked examples and problems are included; MATLAB® source code to support the text is available from www.cambridge.org/9780521860963.

A. F. J. Levi is Professor of Electrical Engineering and of Physics and Astronomy at the University of Southern California. He joined USC in 1993 after working for 10 years at AT & T Bell Laboratories, New Jersey. He invented hot electron spectroscopy, discovered ballistic electron transport in transistors, created the first microdisk laser, and carried out groundbreaking work in parallel fiber optic interconnect components in computer and switching systems. His current research interests include scaling of ultra-fast electronic and photonic devices, system-level integration of advanced optoelectronic technologies, manufacturing at the nanoscale, and the subject of Adaptive Quantum Design.

Applied Quantum Mechanics

Second Edition

A. F. J. Levi

CAMBRIDGE
UNIVERSITY PRESS

CAMBRIDGE UNIVERSITY PRESS
Cambridge, New York, Melbourne, Madrid, Cape Town, Singapore, São Paulo

Cambridge University Press
The Edinburgh Building, Cambridge CB2 2RU, UK

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

www.cambridge.org
Information on this title: www.cambridge.org/9780521860963

First published 2003
Second edition published 2006

Printed in the United Kingdom at the University Press, Cambridge

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

ISBN-13 978-0-521-86096-3 hardback
ISBN-10 0-521-86096-2 hardback

Dass ich erkenne, was die Welt
Im Innersten zusammenhält

Goethe
(*Faust*, I.382–3)

Contents

Preface to the first edition			*page* xiii
Preface to the second edition			xv
MATLAB® programs			xvi
1	**Introduction**		**1**
1.1	Motivation		1
1.2	Classical mechanics		4
	1.2.1	Introduction	4
	1.2.2	The one-dimensional simple harmonic oscillator	7
	1.2.3	Harmonic oscillation of a diatomic molecule	10
	1.2.4	The monatomic linear chain	13
	1.2.5	The diatomic linear chain	15
1.3	Classical electromagnetism		18
	1.3.1	Electrostatics	18
	1.3.2	Electrodynamics	24
1.4	Example exercises		39
1.5	Problems		53
2	**Toward quantum mechanics**		**57**
2.1	Introduction		57
	2.1.1	Diffraction and interference of light	58
	2.1.2	Black-body radiation and evidence for quantization of light	62
	2.1.3	Photoelectric effect and the photon particle	64
	2.1.4	Secure quantum communication	66
	2.1.5	The link between quantization of photons and other particles	70
	2.1.6	Diffraction and interference of electrons	71
	2.1.7	When is a particle a wave?	72
2.2	The Schrödinger wave equation		73
	2.2.1	The wave function description of an electron in free space	79
	2.2.2	The electron wave packet and dispersion	80
	2.2.3	The hydrogen atom	83
	2.2.4	Periodic table of elements	89
	2.2.5	Crystal structure	93
	2.2.6	Electronic properties of bulk semiconductors and heterostructures	96

2.3 Example exercises 103
2.4 Problems 114

3 Using the Schrödinger wave equation 117
3.1 Introduction 117
3.1.1 The effect of discontinuity in the wave function and its slope 118
3.2 Wave function normalization and completeness 121
3.3 Inversion symmetry in the potential 122
3.3.1 One-dimensional rectangular potential well with infinite barrier energy 123
3.4 Numerical solution of the Schrödinger equation 126
3.5 Current flow 128
3.5.1 Current in a rectangular potential well with infinite barrier energy 129
3.5.2 Current flow due to a traveling wave 131
3.6 Degeneracy as a consequence of symmetry 131
3.6.1 Bound states in three dimensions and degeneracy of eigenvalues 131
3.7 Symmetric finite-barrier potential 133
3.7.1 Calculation of bound states in a symmetric finite-barrier potential 135
3.8 Transmission and reflection of unbound states 137
3.8.1 Scattering from a potential step when $m_1 = m_2$ 138
3.8.2 Scattering from a potential step when $m_1 \neq m_2$ 140
3.8.3 Probability current density for scattering at a step 141
3.8.4 Impedance matching for unity transmission across a potential step 142
3.9 Particle tunneling 145
3.9.1 Electron tunneling limit to reduction in size of CMOS transistors 149
3.10 The nonequilibrium electron transistor 150
3.11 Example exercises 155
3.12 Problems 168

4 Electron propagation 171
4.1 Introduction 171
4.2 The propagation matrix method 172
4.3 Program to calculate transmission probability 177
4.4 Time-reversal symmetry 178
4.5 Current conservation and the propagation matrix 180
4.6 The rectangular potential barrier 182
4.6.1 Transmission probability for a rectangular potential barrier 182
4.6.2 Transmission as a function of energy 185
4.6.3 Transmission resonances 186
4.7 Resonant tunneling 188
4.7.1 Heterostructure bipolar transistor with resonant tunnel-barrier 190
4.7.2 Resonant tunneling between two quantum wells 192

4.8 The potential barrier in the delta function limit 197
4.9 Energy bands in a periodic potential 199
4.9.1 Bloch's Theorem 200
4.9.2 The propagation matrix applied to a periodic potential 201
4.9.3 The tight binding approximation 207
4.9.4 Crystal momentum and effective electron mass 209
4.10 Other engineering applications 213
4.11 The WKB approximation 214
4.11.1 Tunneling through a high-energy barrier of finite width 215
4.12 Example exercises 217
4.13 Problems 234

5 Eigenstates and operators 238
5.1 Introduction 238
5.1.1 The postulates of quantum mechanics 238
5.2 One-particle wave function space 239
5.3 Properties of linear operators 240
5.3.1 Product of operators 241
5.3.2 Properties of Hermitian operators 241
5.3.3 Normalization of eigenfunctions 243
5.3.4 Completeness of eigenfunctions 243
5.3.5 Commutator algebra 244
5.4 Dirac notation 245
5.5 Measurement of real numbers 246
5.5.1 Expectation value of an operator 247
5.5.2 Time dependence of expectation value 248
5.5.3 Uncertainty of expectation value 249
5.5.4 The generalized uncertainty relation 253
5.6 The no cloning theorem 255
5.7 Density of states 256
5.7.1 Density of electron states 256
5.7.2 Calculating density of states from a dispersion relation 263
5.7.3 Density of photon states 264
5.8 Example exercises 266
5.9 Problems 277

6 The harmonic oscillator 280
6.1 The harmonic oscillator potential 280
6.2 Creation and annihilation operators 282
6.2.1 The ground state of the harmonic oscillator 284
6.2.2 Excited states of the harmonic oscillator and normalization of eigenstates 287
6.3 The harmonic oscillator wave functions 291
6.3.1 The classical turning point of the harmonic oscillator 295
6.4 Time dependence 298
6.4.1 The superposition operator 300

6.4.2 Measurement of a superposition state 300
6.4.3 Time dependence of creation and annihilation operators 301
6.5 Quantization of electromagnetic fields 305
6.5.1 Laser light 306
6.5.2 Quantization of an electrical resonator 306
6.6 Quantization of lattice vibrations 307
6.7 Quantization of mechanical vibrations 308
6.8 Example exercises 309
6.9 Problems 323

7 Fermions and bosons 326
7.1 Introduction 326
7.1.1 The symmetry of indistinguishable particles 327
7.2 Fermi–Dirac distribution and chemical potential 334
7.2.1 Writing a computer program to calculate the chemical potential 337
7.2.2 Writing a computer program to plot the Fermi–Dirac distribution 338
7.2.3 Fermi–Dirac distribution function and thermal equilibrium statistics 339
7.3 The Bose–Einstein distribution function 342
7.4 Example exercises 343
7.5 Problems 351

8 Time-dependent perturbation 353
8.1 Introduction 353
8.1.1 An abrupt change in potential 354
8.1.2 Time-dependent change in potential 356
8.2 First-order time-dependent perturbation 359
8.2.1 Charged particle in a harmonic potential 360
8.3 Fermi's golden rule 363
8.4 Elastic scattering from ionized impurities 366
8.4.1 The coulomb potential 369
8.4.2 Linear screening of the coulomb potential 375
8.5 Photon emission due to electronic transitions 384
8.5.1 Density of optical modes in three-dimensions 384
8.5.2 Light intensity 385
8.5.3 Background photon energy density at thermal equilibrium 385
8.5.4 Fermi's golden rule for stimulated optical transitions 385
8.5.5 The Einstein $\mathcal{A}$ and $\mathcal{B}$ coefficients 387
8.6 Example exercises 393
8.7 Problems 407

9 The semiconductor laser 412
9.1 Introduction 412
9.2 Spontaneous and stimulated emission 413
9.2.1 Absorption and its relation to spontaneous emission 416

9.3 Optical transitions using Fermi's golden rule 419
9.3.1 Optical gain in the presence of electron scattering 420
9.4 Designing a laser diode 422
9.4.1 The optical cavity 422
9.4.2 Mirror loss and photon lifetime 428
9.4.3 The Fabry–Perot laser diode 429
9.4.4 Semiconductor laser diode rate equations 430
9.5 Numerical method of solving rate equations 434
9.5.1 The Runge–Kutta method 435
9.5.2 Large-signal transient response 437
9.5.3 Cavity formation 438
9.6 Noise in laser diode light emission 440
9.7 Why our model works 443
9.8 Example exercises 443
9.9 Problems 449

10 Time-independent perturbation 450
10.1 Introduction 450
10.2 Time-independent nondegenerate perturbation 451
10.2.1 The first-order correction 452
10.2.2 The second-order correction 453
10.2.3 Harmonic oscillator subject to perturbing potential in x 456
10.2.4 Harmonic oscillator subject to perturbing potential in x^2 458
10.2.5 Harmonic oscillator subject to perturbing potential in x^3 459
10.3 Time-independent degenerate perturbation 461
10.3.1 A two-fold degeneracy split by time-independent perturbation 462
10.3.2 Matrix method 462
10.3.3 The two-dimensional harmonic oscillator subject to perturbation in xy 465
10.3.4 Perturbation of two-dimensional potential with infinite barrier energy 467
10.4 Example exercises 471
10.5 Problems 482

11 Angular momentum and the hydrogenic atom 485
11.1 Angular momentum 485
11.1.1 Classical angular momentum 485
11.2 The angular momentum operator 487
11.2.1 Eigenvalues of angular momentum operators $\hat{L}_z$ and $\hat{L}^2$ 489
11.2.2 Geometrical representation 491
11.2.3 Spherical coordinates and spherical harmonics 492
11.2.4 The rigid rotator 498
11.3 The hydrogen atom 499
11.3.1 Eigenstates and eigenvalues of the hydrogen atom 500
11.3.2 Hydrogenic atom wave functions 508

11.3.3	Electromagnetic radiation	509
11.3.4	Fine structure of the hydrogen atom and electron spin	515
11.4	Hybridization	516
11.5	Example exercises	517
11.6	Problems	529
Appendix A	*Physical values*	532
Appendix B	*Coordinates, trigonometry, and mensuration*	537
Appendix C	*Expansions, differentiation, integrals, and mathematical relations*	540
Appendix D	*Matrices and determinants*	546
Appendix E	*Vector calculus and Maxwell's equations*	548
Appendix F	*The Greek alphabet*	551
Index		552

Preface to the first edition

The theory of quantum mechanics forms the basis for our present understanding of physical phenomena on an atomic and sometimes macroscopic scale. Today, quantum mechanics can be applied to most fields of science. Within engineering, important subjects of practical significance include semiconductor transistors, lasers, quantum optics, and molecular devices. As technology advances, an increasing number of new electronic and opto-electronic devices will operate in ways which can only be understood using quantum mechanics. Over the next thirty years, fundamentally quantum devices such as single-electron memory cells and photonic signal processing systems may well become commonplace. Applications will emerge in any discipline that has a need to understand, control, and modify entities on an atomic scale. As nano- and atomic-scale structures become easier to manufacture, increasing numbers of individuals will need to understand quantum mechanics in order to be able to exploit these new fabrication capabilities. Hence, one intent of this book is to provide the reader with a level of understanding and insight that will enable him or her to make contributions to such future applications, whatever they may be.

The book is intended for use in a one-semester introductory course in applied quantum mechanics for engineers, material scientists, and others interested in understanding the critical role of quantum mechanics in determining the behavior of practical devices. To help maintain interest in this subject, I felt it was important to encourage the reader to solve problems and to explore the possibilities of the Schrödinger equation. To ease the way, solutions to example exercises are provided in the text, and the enclosed CD-ROM contains computer programs written in the MATLAB language that illustrate these solutions. The computer programs may be usefully exploited to explore the effects of changing parameters such as temperature, particle mass, and potential within a given problem. In addition, they may be used as a starting point in the development of designs for quantum mechanical devices.

The structure and content of this book are influenced by experience teaching the subject. Surprisingly, existing texts do not seem to address the interests or build on the computing skills of today's students. This book is designed to better match such student needs.

Some material in the book is of a review nature, and some material is merely an introduction to subjects that will undoubtedly be explored in depth by those interested in pursuing more advanced topics. The majority of the text, however, is an essentially self-contained study of quantum mechanics for electronic and opto-electronic applications.

PREFACE TO THE FIRST EDITION

There are many important connections between quantum mechanics and classical mechanics and electromagnetism. For this and other reasons, Chapter 1 is devoted to a review of classical concepts. This establishes a point of view with which the predictions of quantum mechanics can be compared. In a classroom situation it is also a convenient way in which to establish a uniform minimum knowledge base. In Chapter 2 the Schrödinger wave equation is introduced and used to motivate qualitative descriptions of atoms, semiconductor crystals, and a heterostructure diode. Chapter 3 develops the more systematic use of the one-dimensional Schrödinger equation to describe a particle in simple potentials. It is in this chapter that the quantum mechanical phenomenon of tunneling is introduced. Chapter 4 is devoted to developing and using the propagation matrix method to calculate electron scattering from a one-dimensional potential of arbitrary shape. Applications include resonant electron tunneling and the Kronig-Penney model of a periodic crystal potential. The generality of the method is emphasized by applying it to light scattering from a dielectric discontinuity. Chapter 5 introduces some related mathematics, the generalized uncertainty relation, and the concept of density of states. Following this, the quantization of conductance is introduced. The harmonic oscillator is discussed in Chapter 6 using the creation and annihilation operators. Chapter 7 deals with fermion and boson distribution functions. This chapter shows how to numerically calculate the chemical potential for a multi-electron system. Chapter 8 introduces and then applies time-dependent perturbation theory to ionized impurity scattering in a semiconductor and spontaneous light-emission from an atom. The semiconductor laser diode is described in Chapter 9. Finally, Chapter 10 discusses the (still useful) time-independent perturbation theory.

Throughout this book, I have tried to make applications to systems of practical importance the main focus and motivation for the reader. Applications have been chosen because of their dominant roles in today's technologies. Understanding is, after all, only useful if it can be applied.

A. F. J. Levi
2003

Preface to the second edition

Following the remarkable success of the first edition and not wanting to give up on a good thing, the second edition of this book continues to focus on three main themes: practicing manipulation of equations and analytic problem solving in quantum mechanics, utilizing the availability of modern compute power to numerically solve problems, and developing an intuition for applications of quantum mechanics. Of course there are many books which address the first of the three themes. However, the aim here is to go beyond that which is readily available and provide the reader with a richer experience of the possibilities of the Schrödinger equation and quantum phenomena.

Changes in the second edition include the addition of problems to each chapter. These also appear on the Cambridge University Press website. To make space for these problems and other additions, previously printed listing of MATLAB code has been removed from the text. Chapter 1 now has a section on harmonic oscillation of a diatomic molecule. Chapter 2 has a new section on quantum communication. In Chapter 3 the discussion of numerical solutions to the Schrödinger now includes periodic boundary conditions. The tight binding model of band structure has been added to Chapter 4 and the numerical evaluation of density of states from dispersion relation has been added to Chapter 5. The discussion of occupation number representation for electrons has been extended in Chapter 7. Chapter 11 is a new chapter in which quantization of angular momentum and the hydrogenic atom are introduced.

Cambridge University Press has a website with supporting material for both students and teachers who use the book. This includes MATLAB code used to create figures and solutions to exercises. The website is: http://www.cambrige.org/9780521860963

A. F. J. Levi
2006

MATLAB® programs

The computer requirements for the MATLAB[1] language are an IBM or 100% compatible system equipped with Intel 486, Pentium, Pentium Pro, Pentium4 processor or equivalent. There should be an 8-bit or better graphics adapter and display, a minimum of 32 MB RAM, and at least 50 MB disk space. The operating system should be Windows 95, NT4, Windows 2000, or Windows XP.

If you have not already installed the MATLAB language on your computer, you will need to purchase a copy and do so. MATLAB is available from MathWorks (http://www.mathworks.com/).

After verifying correct installation of MATLAB, download the directory AppliedQMmatlab from www.cambridge.org/9780521860963 and copy to a convenient location in your computer user directory.

Launch MATLAB using the icon on the desktop or from the start menu. The MATLAB command window will appear on your computer screen. From the MATLAB command window use the path browser to set the path to the location of the AppliedQMmatlab directory. Type the name of the file you wish to execute in the MATLAB command window (do not include the ".m" extension). Press the enter key on the keyboard to run the program.

You will find that some programs prompt for input from the keyboard. Most programs display results graphically with intermediate results displayed in the MATLAB command window.

To edit values in a program or to edit the program itself double-click on the file name to open the file editor.

You should note that the computer programs in the AppliedQMmatlab directory are not optimized. They are written in a very simple way to minimize any possible confusion or sources of error. The intent is that these programs be used as an aid to the study of applied quantum mechanics. When required, integration is performed explicitly, and in the simplest way possible. However, for exercises involving matrix diagonalization use is made of special MATLAB functions.

Some programs make use of the functions chempot.m, fermi.m, mu.m, runge4.m, and solve_schM.m, and Chapt9Exercise5.m reads data from the datainLI.txt data input file.

1. MATLAB is a registered trademark of MathWorks, Inc.