Applied Quantum Mechanics

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A. F. J. Levi is Professor of Electrical and Computer Engineering and Physics and Astronomy, and Chair of the Ming Hsieh Department of Electrical and Computer Engineering – Electrophysics, at the University of Southern California (USC). He joined USC after a decade at AT&T Bell Laboratories, Murray Hill, New Jersey, and has over 25 years' experience in teaching applied quantum mechanics to engineers and scientists. He is the inventor of hot electron spectroscopy, discovered ballistic electron transport in transistors, created the first microdisk laser, and carried out groundbreaking work in optimal design of small electronic and photonic systems.

> "Applied Quantum Mechanics, third edition, by A. F. J. Levi, is an essential update in the rapidly evolving field of quantum mechanics. With a clear and concentrated focus on practical equation manipulation, using computational tools, and an intuitive understanding of applications, this edition skillfully integrates the latest advancements in electronics and quantum engineering. An indispensable resource for students and researchers, it strikes the perfect balance between conciseness and comprehensiveness."

Daryoosh Vashaee, North Carolina State University

"The new third edition of this textbook provides an essential introduction to quantum mechanics and its many technological and scientific applications that I would recommend to all undergraduate students. In particular, the focus on technological applications and devices and the many worked example problems make the material more concrete and illustrate the power of quantum mechanics."

Aaron M. Lindenberg, Stanford University

"Applied Quantum Mechanics by Levi stands out because of its unique blend of subjects, encompassing both fundamental and applied aspects of quantum mechanics. The new edition incorporates the subject of quantum circuits and information, which is absolutely timely and highly needed. I have used the previous editions over the years and I look forward to using the new edition. The textbook is especially well suited for upper-class undergraduates and/or first-year graduate students pursuing degrees in engineering or natural sciences."

Ridwan Sakidja, Missouri State University

"This third edition of *Applied Quantum Mechanics* by A. F. J. Levi will be a great asset for students in physics, engineering, and materials science who seek a solid introduction to the practical aspect of quantum mechanics that will allow them to investigate the electrical and optical properties of nanoscale devices. The addition of the section on quantum information processing will also give the students a birds-eye view of the rapidly growing field of quantum computing. Quantum engineering is an important breadth of knowledge that any engineer and scientist interested in the working of devices at the nanoscale must acquire, and this book offers a solid introduction to it."

Marc Cahay, University of Cincinnati

Applied Quantum Mechanics

Third Edition

A. F. J. Levi University of Southern California





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> Dass ich erkenne, was die Welt Im Innersten zusammenhält

> > Goethe (Faust, I.382–3)

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Preface to the Third Edition

A great deal of progress has been made in applied quantum mechanics since the first and second editions of this book were published. While there is a continued focus on three main themes – practicing manipulation of equations and analytic problem solving in quantum mechanics, utilizing the availability of modern computer power to numerically solve problems, and developing an intuition for applications of quantum mechanics – the need for an accessible introductory book about applied quantum mechanics is even greater now than it was in 2003. In the US there is renewed emphasis on research in electronics, particularly transistors and photonics, quantum information processing, and quantum engineering. The third edition of *Applied Quantum Mechanics* sets out to address these interests. To accommodate a new chapter called "Toward Quantum Engineering," the previous first chapter – introducing background material on classical mechanics and electromagnetism – has been moved to an appendix. In addition, the text in the book has been made more concise. This has created room for some additional material whose aim is to maintain reader interest by broadening the range of applications and concepts.

The book content remains designed for a one-semester course. For those on a quarter system or those wishing to focus on core elements of the book, Chapter 9 on time-independent perturbation theory and Chapter 10 on the hydrogen atom can be skipped.

Changes in the third edition include the addition of problems to each chapter. Chapter 11 is new and addresses device optimization, control, and provides an introduction to quantum information processing.

Cambridge University Press has a website with supporting material for both students and instructors who use the book. This includes MATLAB code used to create figures and solutions to exercises. The website is: www.cambridge.org/Levi3e.

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: www.cambridge.org/9780521860963

Many thanks to Omid Nohadani for help with formatting the current version of the book.

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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.

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

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Preface to the First Edition

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

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Note on MATLAB Programs

If you have not already installed the MATLAB^{(B)1} language on your computer, you will need to purchase a copy and do so. MATLAB is available from MathWorks (www.mathworks.com/).

After verifying that MATLAB has been correctly installed, download the directory AppliedQMmatlab from www.cambridge.org/Levi3e 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.

¹ MATLAB is a registered trademark of MathWorks, Inc.

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