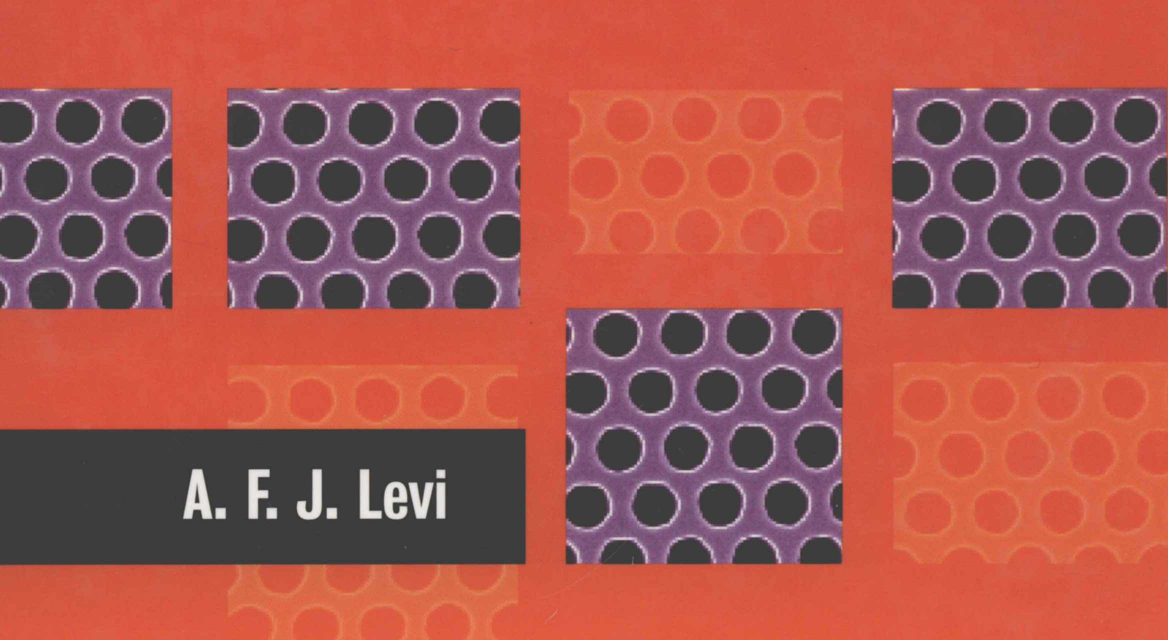
Applied Quantum Mechanics



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. . . Dass ich erkenne, was die Welt
Im Innersten zusammenhält . . .

GOETHE

(Faust. I 382–384)

Preface

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 30 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 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 made 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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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. A CD-ROM drive is required for software installation. There needs to 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 is Windows95, NT4, Windows2000, or WindowsXP.

If you have not already installed MATLAB, you will need to purchase a copy and install it on your computer.

After verifying correct installation of the MATLAB application program, copy the directory AppliedQMmatlab on the CD-ROM to a convenient location in your computer user directory.

Launch the MATLAB application program using the icon on the desktop or from the start menu. The MATLAB command window will appear in 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, solve_schM.m, and Chapt9Exercise5.m reads data from the datainLI.txt data input file.

[1] MATLAB is a registered trademark of the MathWorks, Inc.

Contents

1 Introduction

1.1 Motivation

You may ask why one needs to know about quantum mechanics. Possibly the simplest answer is that we live in a quantum world! Engineers would like to make and control electronic, opto-electronic, and optical devices on an atomic scale. In biology there are molecules and cells we wish to understand and modify on an atomic scale. The same is true in chemistry, where an important goal is the synthesis of both organic and inorganic compounds with precise atomic composition and structure. Quantum mechanics gives the engineer, the biologist, and the chemist the tools with which to study and control objects on an atomic scale.

As an example, consider the deoxyribonucleic acid (DNA) molecule shown in Fig. 1.1. The number of atoms in DNA can be so great that it is impossible to track the position and activity of every atom. However, suppose we wish to know the effect a particular site (or neighborhood of an atom) in a single molecule has on a chemical reaction. Making use of quantum mechanics, engineers, biologists, and chemists can work together to solve this problem. In one approach, laser-induced fluorescence of a fluorophore attached to a specific site of a large molecule can be used to study the dynamics of that individual molecule. The light emitted from the fluorophore acts as a small beacon that provides information about the state of the molecule. This technique, which relies on *quantum mechanical photon stimulation and photon emission from* atomic states, has been used to track the behavior of single DNA molecules.[1]

Interdisciplinary research that uses quantum mechanics to study and control the behavior of atoms is, in itself, a very interesting subject. However, even within a given discipline such as electrical engineering, there are important reasons to study quantum mechanics. In the case of electrical engineering, one simple motivation is the fact that transistor dimensions will soon approach a size where single-electron and quantum effects determine device performance. Over the last few decades advances in the complexity and performance of complementary metal-oxide–semiconductor (CMOS)

[1] S. Weiss, *Science* **283**, 1676 (1999).

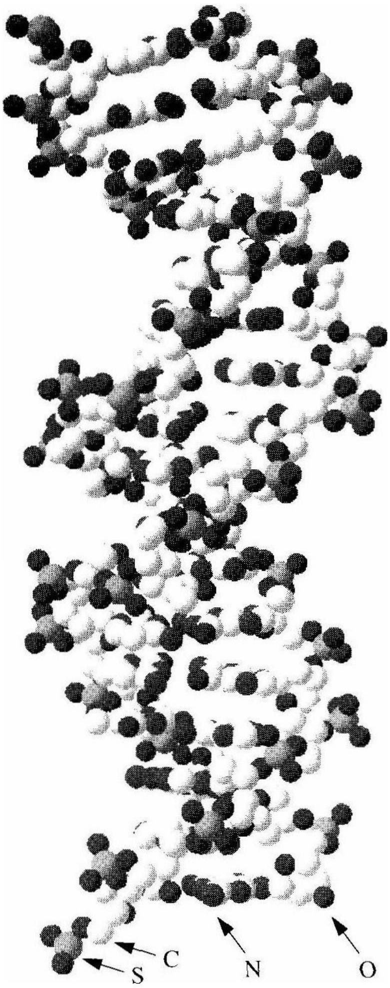

Fig. 1.1. Ball and stick model of a DNA molecule. Atom types are indicated.

circuits have been carefully managed by the microelectronics industry to follow what has become known as "Moore's law".[2] This rule-of-thumb states that the number of transistors in silicon integrated circuits increases by a factor of 2 every 18 months. Associated with this law is an increase in the performance of computers. The Semiconductor Industry Association (SIA) has institutionalized Moore's Law via the "SIA Roadmap", which tracks and identifies advances needed in most of the electronics industry's technologies.[3] Remarkably, reductions in the size of transistors and related technology have allowed Moore's law to be sustained for over 35 years (see Fig. 1.2). Nevertheless, the impossibility of continued reduction in transistor device dimensions is well illustrated by the fact that Moore's law predicts that dynamic random access memory (DRAM)

[2] G. E. Moore, *Electronics* **38**, 114 (1965). Also reprinted in *Proc. IEEE* **86**, 82 (1998).
[3] http://www.sematech.org.

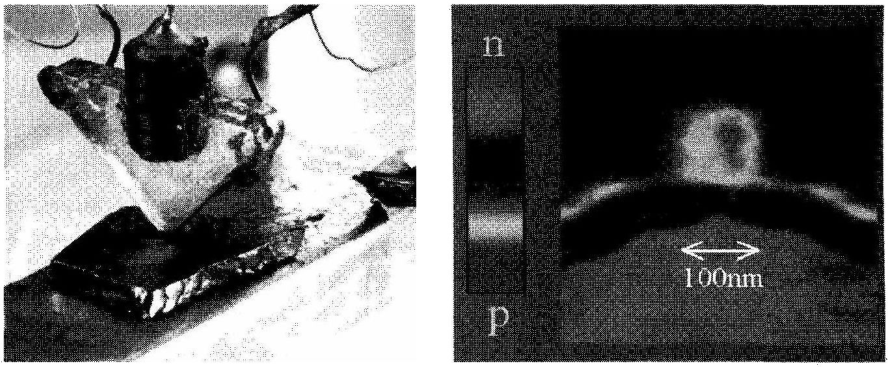

Fig. 1.2. Photograph (left) of the first transistor. Brattain and Bardeen's *p–n–p* point-contact germanium transistor operated as a speech amplifier with a power gain of 18 on December 23, 1947. The device is a few millimeters in size. On the right is a scanning capacitance microscope cross-section image of a silicon *p*-type metal-oxide–semiconductor field-effect transistor (*p*-MOSFET) with an effective channel length of about 20 nm, or about 60 atoms.[4] This image of a small transistor was published in 1998, 50 years after Brattain and Bardeen's device. Image courtesy of G. Timp, University of Illinois.

cell size will be *less* than that of an atom by the year 2030. Well before this end-point is reached, quantum effects will dominate device performance, and conventional electronic circuits will fail to function.

We need to learn to use quantum mechanics to make sure that we can create the smallest, highest-performance devices possible.

Quantum mechanics is the basis for our present understanding of physical phenomena on an atomic scale. Today, quantum mechanics has numerous applications in engineering, including semiconductor transistors, lasers, and quantum optics. As technology advances, an increasing number of new electronic and opto-electronic devices will operate in ways that can only be understood using quantum mechanics. Over the next 20 years, fundamentally quantum devices such as single-electron memory cells and photonic signal processing systems may well become available. It is also likely that entirely new devices, with functionality based on the principles of quantum mechanics, will be invented. The purpose of this book is to provide the reader with a level of understanding and insight that will enable him or her to appreciate and to make contributions to the development of these future, as yet unknown, applications of quantum phenomena.

The small glimpse of our quantum world that this book provides reveals significant differences from our everyday experience. Often we will discover that the motion of objects does not behave according to our (classical) expectations. A simple, but hopefully motivating, example is what happens when you throw a ball against a wall.

[4] Also see G. Timp et al. *IEEE International Electron Devices Meeting (IEDM) Technical Digest* p. 615, Dec. 6–9, San Francisco, California, 1998 (ISBN 0780 3477 9).

Of course, we expect the ball to bounce right back. Quantum mechanics has something different to say. There is, under certain special circumstances, a finite chance that the ball will appear on the other side of the wall! This effect, known as tunneling, is fundamentally quantum mechanical and arises due to the fact that on appropriate time and length scales particles can be described as waves. Situations in which *elementary* particles such as electrons and photons tunnel are, in fact, relatively common. However, quantum mechanical tunneling is not always limited to atomic-scale and elementary particles. Tunneling of *large* (macroscopic) objects can also occur! Large objects, such as a ball, are made up of many atomic-scale particles. The possibility that such large objects can tunnel is one of the more amazing facts that emerges as we explore our quantum world.

However, before diving in and learning about quantum mechanics it is worth spending a little time and effort reviewing some of the basics of classical mechanics and classical electromagnetics. We do this in the next two sections. The first deals with classical mechanics, which was first placed on a solid theoretical basis by the work of Newton and Leibniz published at the end of the seventeenth century. The survey includes reminders about the concepts of potential and kinetic energy and the conservation of energy in a closed system. The important example of the one-dimensional harmonic oscillator is then considered. The simple harmonic oscillator is extended to the case of the diatomic linear chain, and the concept of dispersion is introduced. Going beyond mechanics, in the following section classical electromagnetism is explored. We start by stating the coulomb potential for charged particles, and then we use the equations that describe electrostatics to solve practical problems. The classical concepts of capacitance and the coulomb blockade are used as examples. Continuing our review, Maxwell's equations are used to study electrodynamics. The first example discussed is electromagnetic wave propagation at the speed of light in free space, c. The key result – that power and momentum are carried by an electromagnetic wave – is also introduced.

Following our survey of classical concepts, in Chapter 2 we touch on the experimental basis for quantum mechanics. This includes observation of interference phenomenon with light, which is described in terms of the linear superposition of waves. We then discuss the important early work aimed at understanding the measured power spectrum of black-body radiation as a function of wavelength, λ, or frequency, $\omega = 2\pi c/\lambda$. Next, we treat the photoelectric effect, which is best explained by requiring that light be quantized into particles (called photons) of energy $E = \hbar\omega$. Planck's constant $\hbar = 1.0545 \times 10^{-34}$ J s, which appears in the expression $E = \hbar\omega$, is a small number that sets the absolute scale for which quantum effects usually dominate behavior.[5] Since the typical length scale for which electron energy quantization is important usually turns out to be the size of an atom, the observation of discrete spectra for light emitted from excited atoms is an effect that can only be explained using quantum mechanics.

[5] Sometimes $\hbar$ is called Planck's *reduced* constant to distinguish it from $h = 2\pi\hbar$.