Peter Deák

Essential Quantum Mechanics for Electrical Engineers

 $E_n = \frac{n^2}{8mL^2}(n+1)^2; n = 0, 1.$

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WILEY-VCH

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Cover

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Library of Congress Card No.: applied for

British Library Cataloguing-in-Publication Data

A catalogue record for this book is available from the British Library.

Bibliographic information published by theDeutsche Nationalbibliothek

The Deutsche Nationalbibliothek lists this publication in the Deutsche Nationalbibliografie; detailed bibliographic data are available on the Internet at http://dnb.d-nb.de.

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Print ISBN: 978-3-527-41355-3 ePDF ISBN: 978-3-527-80581-5 ePub ISBN: 978-3-527-80583-9 Mobi ISBN: 978-3-527-80584-6

Cover Design Bluesea Design, McLeese Lake, Canada Typesetting SPi Global Private Limited, Chennai, India Printing and Binding

Printed on acid-free paper

For my children and grandchildren.

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Preface

My motivation for writing this book was the expected effect of nanotechnology on engineering, which will surely and significantly enhance the demand for the knowledge of quantum mechanics (QM). Although present-day micro- and optoelectronics can, to a degree, be understood using semiclassical models, this situation is going to change soon. The limits of development in the traditional (twentieth century) hardware have almost been reached. The upcoming devices – where switching happens at the level of single electrons, tunnel effects are actively utilized, and superposition states of electrons are used as qubits – are based on phenomena that cannot be grasped even approximately without the conceptual understanding of QM. Most students graduating in electrical engineering in the coming years will definitely be confronted in their professional career with the paradigm shift induced by the new technologies of the quantum world. This explains why the teaching of QM should begin early.

Although teaching QM to students of electrical engineering (and informatics) at the undergraduate level is becoming more and more widespread, there are hardly any textbooks written specifically for such courses. Typical books on QM are not well suited for engineers because of the excessive use of mathematics and because of the very abstract way of treatment with little or no applications relevant to them. QM books written for electrical engineers are usually either resorting to heuristics or aim at the band theory of solids (to be able to describe semiconductor applications), the latter being well beyond the possibilities provided by a bachelor curriculum. Based on my 25 years of experience in teaching QM for undergraduate students of electrical engineering and informatics, I have attempted to write a textbook, adjusted to their knowledge level and interests, which can be the basis of a two hours a week, one semester course.

From the viewpoint of electrical engineering, QM is primarily the physics of electrons. Its knowledge enables us to use them for information processing, storage, and display, as well as for lighting and energy production. Our organs of perception cannot register individual electrons, so we cannot really *imagine* what they are really like. As Richard Feynman has formulated it, the electron is not an object (what we can see or hold) but a concept, which can only be formulated mathematically. Accordingly, QM can only be formulated and interpreted mathematically, and this seems to be, at the first sight to undergraduates in electrical engineering, rather difficult to digest and of little practical interest. However,

information technology is an important part of the trade, and the physics necessary to understand the hardware of electronic data processing and the conversion between electronic and electromagnetic information in data storage, transfer, and display has become indispensable. The majority of the graduates in electrical engineering and informatics will primarily be interested in system integration and algorithms, but optimal efficiency can only be achieved if they have an at least conceptual understanding about the working of the devices to be integrated and programmed. In addition, QM has changed our perception of reality very much, allowing a much deeper understanding of nature. Therefore, it should be part of the education of anybody striving for a bachelor degree in science and technology.

This book was specifically written for undergraduates of electrical engineering and shows the interlocking between the development of OM and the hardware of lighting technology, opto-, and microelectronics, as well as quantum information processing. I have attempted to demonstrate the surprising claims of basic QM in direct applications. The "Introduction" summarizes the basic concepts of classical physics and points out some of its failures, based on phenomena connected to lighting technology. These (blackbody radiation in the light bulb, emission spectrum of the gas fill, and cathode emission in discharge lamps) are analyzed in detail in Chapters 2-4, based on experiments which are famous in physics. It is shown that a surprising but rather controversial first explanation of the results could be provided in terms of the wave-particle duality principle. The use of that by Einstein led later to the discovery of the laser (which is also described). Chapter 5 goes beyond the duality principle and explains the particle concept of the QM and its consequences for electrical engineering (e.g., negative differential resistivity). Chapters 6-8 introduce the mathematical construction used for describing the state of a particle and to predict its properties. In Chapters 9 and 10, two examples of using this framework are shown (potential well and tunneling through a potential barrier), with applications, among others, in light-emitting diodes, infrared detectors, quantum cascade lasers, Zener diodes, and flash memories. The scanning tunneling microscope is, of course, explained and also the leakage currents in integrated circuits and the electric breakdown of insulators. Finally, in Chapters 11 and 12, some consequences of the QM for the chemical properties of atoms and for other many-electron systems (such as semiconductors) are depicted, giving also a brief insight into the potential hardware for quantum information processing. In Appendices A and B, the knowledge in classical physics and mathematics is summarized, which is a prerequisite to read the book. (It is strongly recommended to work through these appendices first.)

This book attempts to choose a middle course between abstract mathematics and applications. On the one hand, basic concepts and principles of the QM are introduced in the necessary mathematical formulation, but the mathematics is kept as simple as possible. Only those tools of advanced mathematics are used, which have to be learned in the electronic engineering curriculum anyhow, and even they are used to treat specific cases relevant for applications. Engineers usually prefer ready-made formulas over mathematical derivation. However, since the internal logic of QM is actually in the derivations, the most important ones are shown in this book – but only as footnotes. Chapters 9 and 10 are the two exceptions from this rule, where practically applicable formulas can be derived in elementary steps, helping the reader to gain a deeper understanding of specific cases. In addition, knowing very well that the targeted readers are mostly not too mathematics oriented, the book exploits the possibilities of multimedia: besides numerous figures and pictures, video clips and applets, accessible on the Internet, are used intensively. Application of QM often requires serious efforts with numerical calculations, but applets can ease the burden of that, allowing quick visualization of trends and easier cognition of graphically displayed information.

Finally, it should be noted that QM has raised many philosophical, epistemological questions. As far as possible, these have been swept under the carpet in this book, and – to use a philosophical term – a rather positivistic representation was chosen. Since this book was written for engineers, prediction of practical results should take precedence over philosophical interpretation. In addition, it is probably better to get a simplified but applicable picture, which later can be refined, than being bogged down right at the beginning with interpretational controversies.

I would like to express my gratitude to the people who have helped me to complete this book: Dr Bálint Aradi and Dr Michael Lorke, who have read and corrected the original German version, and Prof. Japie Engelbrecht who did the same with this English one.

Bremen 2016

Peter Deák

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Introduction: Classical Physics and the Physics of Information Technology

This chapter...

describes the view of classical physics about matter. The knowledge developed from these concepts has led to the first industrial revolution; however, it is not sufficient to explain many of the present technologies. The need for a substantial extension of physics is demonstrated by following the development of lighting technology.

1

1.1 The Perception of Matter in Classical Physics: Particles and Waves

The task of physics is the description of the state and motion of matter in a mathematical form, which allows quantitative predictions based on known initial conditions. Mathematical relationships are established for simplified and idealized model systems. Classical physics considers two basic forms of matter: *bodies* and *radiation*, characterized by mass *m* and energy *E*, respectively. The special relativity theory of Einstein (see Section A.9) has established that these two forms of matter can be mutually transformed into each other. In nuclear fusion or fission, for example, part of the initial mass will be converted into electromagnetic (EM) radiation (in the full spectral range from heat to X-rays), while energetic EM radiation can produce electron–positron pairs. The equivalence of mass and energy is expressed by $E = mc^2$. Still, the models used for the two forms of matter are quite different.

In classical physics, radiation is a *wave* in the ideally elastic continuum of the infinite EM field. Waves are characterized by their (angular) frequency ω and wave number k. These quantities are not independent, and the so-called dispersion relation between them, $\omega = \omega(k)$, determines the phase velocity v_f and group velocity v_g of the wave (see Sections A.5 and A.6). The energy of the wave is $E \sim v_f |E_0|^2$, where E_0 is the amplitude of the EM wave.

In contrast to the continuous EM field, bodies consist of discrete *particles*. The fundamental building blocks are the elementary particles¹ listed in Table 1.1.

1

¹ Solids, fluids, and gases all consist of atoms with a nucleus and electrons. The nucleus consists of protons and neutrons, both of which are made up of quarks.

2 1 Introduction: Classical Physics and the Physics of Information Technology

Particles	First generation	Second generation	Third generation
Quarks	Up (u)	Charm (C)	Top (t)
	Down (d)	Strange (S)	Bottom (b)
Leptons	Electron (e)	Muon (µ)	Tau (τ)
	e-Neutrino	μ-Neutrino	au-Neutrino

Table 1.1 The elementary particles.

The model of classical physics for particles is the *point mass*: a geometrical point (with no extension in space) containing all the mass of the particle. It has been found that the center of mass of an extended body is moving in such a way as if all the mass was carried by it, and all the forces were acting on it. Therefore, the concept of the point mass can even be applied for extended bodies. The point mass can be characterized by its position in space (r) and by its velocity (v), both of which can be accurately determined as functions of time. These kinematic quantities are then used to define the dynamic quantities, *momentum* p, *angular momentum* L, and *kinetic energy* T (see Section A.3).

The laws and equations of classical physics are formulated for point-mass-like particles and for waves in an infinite medium.

1.2 Axioms of Classical Physics

The motion of interacting point masses can be described by the help of the four Newtonian axioms (see Section A.2), which allow the writing down of an equation of motion for each point mass. Unfortunately, this system of equations can only be solved if the number of point masses is small or if we can assume that the distance between them is constant (rigid bodies). If the number of particles is high and the interaction between them is weak, a model of noninteracting particles (ideal gas) can be applied, and the system can be described by thermo-dynamic state variables. The changes in these are governed by the four laws of thermodynamics and by the equation of state. Actually, the state variables can be expressed by the Newtonian dynamic quantities, and the equation of state, as well as the four laws, can be derived from the Newtonian axioms with the help of the statistical physics and the kinetic gas theory (Figure 1.1).

The behavior of the EM field is described by the four axioms of Maxwell's field theory (see Section A.6). Far away from charges, these give rise to a wave equation, the solutions of which are the EM waves, traveling with the speed of light. The propagation of a local change in the field strength E can be given by the wave function E(r,t). The wave front is defined by the neighboring points in space where E has the same phase. Each point of the wave front is the source of a secondary elementary wave, and the superposition of the latter explains the well-known wave effects of refraction and diffraction.

Elastic and plastic (deformable) bodies (solids and fluids) contain a huge number of interacting particles, and neither the model of rigid bodies nor the model of 1.3 Status and Effect of Classical Physics by the End of the Nineteenth Century 3



Figure 1.1 Models and axioms of classical physics.

the ideal gas can be applied. Instead, a continuum model can be used by assuming a continuous mass distribution, neglecting the corpuscular nature of the body. In the case of elastic bodies, the Newtonian equation for an infinitesimal volume of the continuum leads to a wave equation. The solutions are mechanical waves, corresponding to the propagation of local changes in the position (vibrations). The concepts and mathematics of mechanical and EM waves are quite similar.

1.3 Status and Effect of Classical Physics by the End of the Nineteenth Century

As we have seen in the previous subsection, classical physics contains two relatively independent parts: *mechanics* (from which also the thermodynamics can be derived) and *electrodynamics* (including optics).² Particles in classical mechanics are described by the concept of the point mass. In a conservative force field, where the potential energy V(x,t) can be defined, the position of the point mass can be obtained from the Newtonian equation of motion:

$$m\ddot{x}(t) = \frac{dV(x,t)}{dx}$$
(1.1)

Historically (see Figure 1.2), the concept of the point mass has evolved, among others, from

² More generally, one should talk about field theory. However, as we explain later, the only really relevant force field in electrical engineering is the EM field.