Quantum Mechanics for Scientists and Engineers

If you need a book that relates the core principles of quantum mechanics to modern applications in engineering, physics, and nanotechnology, then *Quantum Mechanics for Scientists and Engineers* is it.

The book's applied emphasis means that the key concepts are introduced in the context of their use in science and technology, with examples of nanostructured materials, optics, and semiconductor devices. Clear explanations of quantum mechanics's basic physics and mathematics, along with algorithms for the computational analysis of simple structures, make this an ideal introductory text. The many worked examples and 160 homework problems help students with problem solving and application of theory. No prior knowledge of high-level physics, difficult mathematics, or classical mechanics is assumed, and supporting math is included in appendices. Students of engineering, physics, nanotechnology, and other disciplines will be able to access more advanced texts on specific aspects of quantum mechanics after using this book.

The text introduces Schrödinger's equation, operators, and approximation methods. Systems, including the hydrogen atom and crystalline materials, are analyzed in detail. More advanced subjects, such as density matrices, quantum optics, and quantum information, are also covered. Online resources include instructor solutions, animations of figures to reinforce key concepts, illustrations, presentation materials, and worked examples. The text's pedagogy and accompanying materials provide a complete teaching package, which clearly develops and delivers one of physics's foundational topics.

Additional resources for this title are available from www.cambridge.org/9780521897839.

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To Pat, Andrew, and Susan

Contents

Preface

This book introduces quantum mechanics to scientists and engineers. It can be used as a text for junior undergraduates onward through to graduate students and professionals. The level and approach are aimed at anyone with a reasonable scientific or technical background looking for a solid but accessible introduction to the subject. The coverage and depth are substantial enough for a first quantum mechanics course for physicists. At the same time, the level of required background in physics and mathematics has been kept to a minimum to suit those from other science and engineering backgrounds.

Quantum mechanics has long been essential for all physicists and for other physical science subjects, such as chemistry. With the growing interest in nanotechnology, quantum mechanics has recently become increasingly important for an ever-widening range of engineering disciplines, such as electrical and mechanical engineering, and for subjects such as materials science that underlie many modern devices. Many physics students also find that they are increasingly motivated in the subject as the everyday applications become clear.

Nonphysicists have a particular problem finding a suitable introduction to the subject. The typical physics quantum mechanics course or text deals with many topics that, though fundamentally interesting, are useful primarily to physicists doing physics; that choice of topics also means omitting many others that are just as truly quantum mechanics but that have more practical applications. Too often, the result is that engineers or applied scientists cannot afford the time or sustain the motivation to follow such a physics-oriented sequence. As a result, they never have a proper grounding in the subject. Instead, they pick up bits and pieces in other courses or texts. Learning quantum mechanics in such a piecemeal approach is especially difficult; students then never properly confront the many fundamentally counterintuitive concepts of the subject. Those concepts need to be understood quite deeply if students are ever going to apply the subject with any reliability in any novel situation. Too often, also, even after working hard in a quantum mechanics class and even after passing the exams, students are still left with the depressing feeling that they do not understand the subject at all.

To address the needs of its broad intended readership, this book differs from most others in three ways. First, it presumes as little as possible in prior knowledge of physics. Specifically, it does not presume the advanced classical mechanics (including concepts such as Hamiltonians and Lagrangians) that is often a prerequisite in physics quantum mechanics texts and courses. Second, in two background appendices, it summarizes all of the key physics and mathematics beyond the high school level that the reader needs to start the subject. Third, it introduces the quantum mechanics that underlies many important areas of application, including semiconductor physics, optics, and optoelectronics. Such areas are usually omitted from quantum mechanics texts, but this book introduces many of the quantum mechanical principles and models that are exploited in those subjects.

It is also my belief and experience that using quantum mechanics in several different and practical areas of application removes many of the difficulties in understanding the subject. If quantum mechanics is illustrated only through examples that are found in the more esoteric

branches of physics, the subject itself can seem irrelevant and obscure. There is nothing like designing a real device with quantum mechanics to make the subject tangible and meaningful.

Even with its deliberately limited prerequisites and its increased discussion of applications, this book offers a solid foundation in the subject. That foundation should well prepare the reader for the quantum mechanics in either advanced physics or deeper study of practical applications in other scientific and engineering fields. The emphasis is on understanding the ideas and techniques of quantum mechanics rather than attempting to cover all possible examples of their use. A key goal of this book is that the reader should subsequently be able to pick up texts in a broad range of areas – including, for example, advanced quantum mechanics for physicists, solid-state and semiconductor physics and devices, optoelectronics, quantum information, and quantum optics – and find they already have all the necessary basic tools and conceptual background in quantum mechanics to make rapid progress.

It is possible to teach quantum mechanics in many different ways, though most sequences will start with Schrödinger's wave equation and work forward from there. Even though the final emphasis in this book may be different from some other quantum mechanics courses, I have deliberately chosen to not take a radical approach here. This is for three reasons: first, most college and university teachers will be most comfortable with a relatively standard approach because that is the one they have most probably experienced themselves; second, taking a core approach that is relatively conventional will make it easier for readers (and teachers) to connect with the many other good physics quantum mechanics books; and third, this book should also be accessible and useful to professionals who have previously studied quantum mechanics to some degree but who need to update their knowledge or connect to the modern applications in engineering or applied sciences.

The background requirements for the reader are relatively modest and should represent little problem for students or professionals in engineering, applied sciences, physics, or other physical sciences. This material has been taught with apparent success to students in applied physics, electrical engineering, mechanical engineering, materials science, and other science and engineering disciplines, from third-year undergraduate level up to the graduate level. In mathematics, readers should have a basic knowledge of calculus, complex numbers, elementary matrix algebra, geometrical vectors, and simple and partial differential equations. In physics, readers should be familiar with ordinary Newtonian classical mechanics and elementary electricity and magnetism. The key requirements are summarized in two background appendices in case readers want to refresh some background knowledge or fill in gaps. A few other pieces of physics and mathematics are introduced as needed in the main body of the text. It is helpful if students have had some prior exposure to elementary modern physics, such as the ideas of electrons, photons, and the Bohr model of the atom, but no particular results are presumed here. The necessary parts of Hamiltonian classical mechanics are introduced briefly when required in later chapters.

This book goes deeper into certain subjects, such as the quantum mechanics of light, than most introductory physics texts. For the later chapters on the quantum mechanics of light, additional knowledge of vector calculus and electromagnetism to the level of Maxwell's equations is presumed, though again these are summarized in appendices.

One intent is for students to acquire a strong understanding of the concepts of quantum mechanics at the level beyond mere mathematical description. As a result, I have chosen to try to explain concepts with limited use of mathematics wherever possible. With the ready availability of computers and appropriate software for numerical calculations and simulations, it is progressively easier to teach principles of quantum mechanics without as heavy an

emphasis on analytical techniques. Such numerical approaches are also closer to the methods that an engineer will likely use for calculations in real problems anyway, and access to some form of computer and high-level software package is assumed for some of the problems. This approach substantially increases the range of problems that can be examined both for tutorial examples and for applications.

Finally, I will make one personal statement on handling the conceptual difficulties of quantum mechanics in texts and courses. Some texts are guilty of stating quantum mechanical postulates, concepts, and assumptions as if they should be obvious, or at least obviously acceptable, when in fact they are far from obvious even to experienced practitioners or teachers. In many cases, these are subjects of continuing debate at the highest level. I try throughout to be honest about those concepts and assumptions whose obviousness or even correctness is genuinely unclear. I believe it is a particularly heinous sin to pretend that some concept should be clear to students when it is, in fact, not even clear to the professor (an overused technique that preserves professorial ego at the expense of the students'!).

It is a pleasure to acknowledge the many teaching assistants who have provided much useful feedback and correction of my errors in this material as I have taught it at Stanford, including Aparna Bhatnagar, Julien Boudet, Eleni Diamanti, Onur Fidaner, Martina Gerken, Noah Helman, Ekin Kocabas, Bianca Nelson, Vincent Revol, Jean-Christophe Richard, Tomas Sarmiento, and Scott Sharpe. I would like to thank Emel Tasyurek for a particularly careful reading of the manuscript, Ingrid Tarien for much help in preparing many parts of the course material, and Marjorie Ford for many helpful comments on writing.

I am also pleased to acknowledge my many professorial colleagues at Stanford, including, in particular, Steve Harris, Walt Harrison, Jelena Vuckovic, and Yoshi Yamamoto for many stimulating, informative, and provocative discussions about quantum mechanics. I would especially like to thank Jelena Vuckovic, who successfully taught the subject to many students despite having to use much of this material as a course reader, and who consequently corrected numerous errors and clarified many points. All remaining errors and shortcomings are, of course, my sole responsibility, and any further corrections and suggestions are most welcome.

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Frontmatter
More Information

How to use this book

For teachers

The entire material in this book could be taught in a one-year course. More likely, depending on the interests and goals of the teacher and students and the length of time available, only some of the more advanced topics will be covered in detail. In a two-quarter course sequence for senior undergraduates and for engineering graduate students at Stanford, the majority of the material here will be covered, with a few topics omitted and some covered in lesser depth.

The core material (Chapters 1–5) on Schrödinger's equation and on the mathematics behind quantum mechanics should be taught in any course. Chapter 4 gives a more explicit introduction to the ideas of linear operators than is found in most texts. Chapter 4 also explains and introduces Dirac notation, which is used from that point onward in the book. This introduction of Dirac notation is earlier than in many older texts, but it saves considerable time thereafter in describing quantum mechanics. Experience teaching engineering students in particular, most of whom are quite familiar with linear algebra and matrices from other applications in engineering, shows that they have no difficulties with this concept.

Aside from that core, there are many possible choices about the sequence of material and about what material needs to be included in a course. The prerequisites for each chapter are clearly stated at the beginning of the chapter. There are also some sections in several of the chapters that are optional or that may only need to be read through when first encountered. These sections are clearly marked. The discussion of methods for one-dimensional problems in Chapter 11 can come at any point after the material on Schrödinger's equations (Chapters 2 and 3). The core transfer matrix part could even be taught directly after the time-independent equation (Chapter 2). The material is optional in that it is not central to later topics, but, in my experience, students usually find it stimulating and empowering to be able to do calculations with simple computer programs based on these methods. This can make students comfortable with the subject and begin to give them some intuitive feel for many quantum mechanical phenomena. (These methods are also used, in practice, for the design of real optoelectronic devices.)

For a broad range of applications, the approximation methods of quantum mechanics (Chapters 6 and 7) are probably the next most important after Chapters 1 through 5. The specific topic of the quantum mechanics of crystalline materials (Chapter 8) is particularly important for many applications and can be introduced at any point after Chapter 7; it is not, however, required for subsequent chapters (except for a few examples and some optional parts at the end of Chapter 11), so teachers can choose how far they want to progress through this chapter. For fundamentals, angular momentum (Chapter 9) and the hydrogen atom (Chapter 10) are the next most central topics, both of which can be taught directly after Chapter 5, if desired. After these, the next most important fundamental topics are spin (Chapter 12) and identical particles (Chapter 13), and these should probably be included in the second quarter or semester, if not before.

Chapter 14 introduces the important technique of the density matrix for connecting to statistical mechanics, and it can be introduced at any point after Chapter 5; preferably, students would also have covered Chapters 6 and 7 so they are familiar with perturbation theory, though that is not required. The density matrix material is not required for subsequent chapters, so Chapter 14 is optional.

The sequence of Chapters 15–17 introduces the quantum mechanics of electromagnetic fields and light as well as the important technique of second quantization in general, including fermion operators (a technique that is also used extensively in more advanced solid-state physics). The inclusion of this material on the quantum mechanics of light is the largest departure from typical introductory quantum mechanics texts. It does, however, redress a balance in material that is important from a practical point of view; we cannot describe even the simplest light emitter (including an ordinary light bulb) or light detector without it, for example. This material is also very substantial quantum mechanics at the next level of the subject. These chapters do require almost all of the preceding material, with the possible exceptions of Chapters 8, 11, and 14.

The final two chapters, Chapter 18 on a brief introduction to quantum information concepts and Chapter 19 on the interpretation of quantum mechanics, could conceivably be presented with only Chapters 1–5 as prerequisites. Preferably also Chapters 9, 10, 12, and 13 would have been covered, and it is probably a good idea that students have been working with quantum mechanics successfully for some time before attempting to grapple with the tricky conceptual and philosophical aspects in these final chapters. The material in these chapters is well suited to the end of a course, when it is often unreasonable to include any further new material in a final exam, but teachers want to keep the students' interest with stimulating ideas.

Problems are introduced directly after the earliest possible sections rather than being deferred to the end of the chapters, thus giving the greatest flexibility in assigning homework. Solutions to selected problems are openly available from www.cambridge.org/9780521897839 (these problems are marked with an asterisk [*] in the text); such problems could be used as additional practice material by students or as worked examples in class. Some of the problems can be used as substantial assignments, and all such problems are clearly marked. These are suitable for "take-home" problems or exams or as extended exercises coupled with tutorial "question-and-answer" sessions. These assignments may necessarily involve some more work, such as significant amounts of (relatively straightforward) algebra or calculations with a computer. I have found, though, that students gain a much greater confidence in the subject once they have used it for something beyond elementary exercises – exercises that are necessarily often artificial. At least, these assignments tend to approach the subject from the point of view of a problem to be solved rather than an exercise that just uses the last technique that was studied. Some of these larger assignments deal with quite realistic uses of quantum mechanics.

At the very end of the book, I also include a suggested list of simple formulae to be memorized in each chapter. These lists could also be used as the basis of simple quizzes or as required learning for "closed-book" exams.

For students

Necessary background

Students will come to this book with very different backgrounds. You may recently have studied a lot of physics and mathematics at the college level. If so, then you are ready to start. I

suggest you have a quick look at Appendices A and B just to see the notations used in this book before starting Chapter 2.

For others, your mathematical or physics background may have been less complete, or it may be some time since you have seen or used some of the relevant parts of these subjects. Rest assured, first of all, that in writing this book I have presumed the least possible knowledge of mathematics and physics consistent with teaching quantum mechanics, and much less than the typical quantum mechanics text requires. Ideally, I expect you have had the physics and mathematics typical of first- or second-year college-level general engineering or physical science students. You do absolutely have to know elementary algebra, calculus, and physics to a good precollege level, however. I suggest you read the Background Mathematics Appendix A and the Background Physics Appendix B to see if you understand most of that. If not too much of that is new to you, then you should be able to proceed into the main body of this book. If you find some new topics in these Appendices, there is, in principle, enough material there to "patch over" those holes in knowledge so that you can use the mathematics and physics needed to start quantum mechanics; Appendices A and B are not, however, meant to be a substitute for learning these topics in greater depth.

Study aids in this book

Lists of concepts introduced

Because there are many concepts that students need to understand in quantum mechanics, I have summarized the most important ones at the end of the chapters in which they are introduced. These summaries should help in both following the "plot" of the book and revising the material.

Appendices

The book is as reasonably self-contained as I can make it. In addition to the background Appendices A and B covering the overall prerequisite mathematics and physics, background material needed later on is introduced in Appendices C and D (vector calculus and electromagnetism), and one specific detailed derivation is given in Appendix E. Appendix F summarizes the early history of quantum mechanics and Appendix G collects and summarizes most of the mathematical formulae that will be needed in the book, including the most useful ones from elementary algebra, trigonometric functions, and calculus. Appendix H gives the Greek alphabet (every single letter of it is used somewhere in quantum mechanics), and Appendix I lists all the relevant fundamental constants.

Problems

There are 160 problems and assignments, collected at the end of the earliest possible sections, rather than at the end of the chapters. Solutions to thirty-six of these are openly available from www.cambridge.org/9780521897839 (these problems are marked with an asterisk [*] in the text), giving additional worked examples for practice or study.

Memorization list

Quantum mechanics, like many aspects of physics, is not primarily about learning large numbers of formulae but rather understanding the key concepts clearly and deeply. It will, however, save a lot of time (including in exams!) to learn a few basic formulae by heart; certainly, if you also understand these well, you should have a good command of the subject.

At the very end of the book, there is a list of formulae worth memorizing in each chapter of the book. None of these formulae are particularly complicated – the most complicated ones are

the two forms of the Schrödinger wave equation. Many of the formulae are simply short definitions of key mathematical concepts. If you learn these formulae chapter-by-chapter as you work through the book, there are not very many formulae to learn at any one time.

The list here is not of the formulae themselves but rather descriptions of them, so you can use this list as an exercise to test how successfully you have learned these key results.

Self-teaching

If you are teaching yourself quantum mechanics using this book, first, congratulations for having the courage to tackle what most people typically regard as a daunting subject. For someone with elementary college-level physics and mathematics, I believe it is quite an accessible subject, in fact. *But*, the most important point is that you must not start learning quantum mechanics "on the fly" by picking and choosing just the bits you need from this book or any other. Trying to learn quantum mechanics like that would be like trying to learn a language by reading a dictionary. You cannot treat quantum mechanics as just a set of formulae to be substituted into problems, just as you cannot translate a sentence from one language to another just by looking up the individual words in a dictionary and writing down their translation. There are just so many counterintuitive aspects about quantum mechanics that you will never understand it in that piecemeal way and, most likely, you would not use the formulae correctly anyway. Make yourself work on all of the first several chapters, through at least Chapter 5; that will get you to a first plateau of understanding. You can be somewhat more selective after that. For the next level of understanding, you need to study angular momentum, spin, and identical particles (Chapters 9, 12, and 13). Which other chapters you use will depend on your interests or needs. Of course, it is worthwhile studying all of them if you have the time!

Especially if you have no tutor of whom you can ask questions, then I also expect that you should be looking at other quantum mechanics books as well. Use this one as your core and, when I have just not managed to explain something clearly enough or to get it to "click" for you, look at some of the others, such as the ones listed in the Bibliography. My personal experience is that a difficult topic finally becomes clear to me once I have five books on it open on my desk. One hope I have for this book is that it enables readers to access the more specialized physics texts, if necessary. Their alternative presentations may well succeed where mine fail, and those other books can certainly cover a range of specific topics impossible to include here.