An Introduction to

Quantum Theory

F. S. Levin

量子理论导论

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An Introduction to Quantum Theory

Underpinning the axiomatic formulation of quantum theory presented in this undergraduate textbook is a review of early experiments, a comparison of classical and quantal terminology, a Schrödinger-equation treatment of the one-dimensional quantum box, and a survey of relevant mathematics. Among the many concepts comprehensively discussed are operators; state vectors, wave functions and their interrelation; experimental observables and their quantum counterparts; classical/quantal connections; and symmetry properties. The theory is applied to a wide variety of systems including the non-relativistic H-atom, external electromagnetic fields, and spin. Collisions are described using wave packets. Various time-dependent and time-independent approximations are discussed; applications include electromagnetic transition rates and corrections to the non-relativistic H-atom energies. The final chapter deals with multiparticle systems and identical-particle symmetries with application to the He-atom, the periodic table, and diatomic molecules. There are also brief treatments of advanced subjects such as gauge invariance, observable phase effects, and hidden variables.

The author received his undergraduate degree from Johns Hopkins University and his Ph.D. from the University of Maryland. Following post-doctoral positions at Rice University, Brookhaven National Laboratory, and the United Kingdom Atomic Energy Authority, he accepted an appointment as a faculty member in the Physics Department at Brown University, where he remained, did research and taught for 31 years until his retirement in 1998. Professor Levin's research areas are nuclear-reaction theory, three-body physics, many-body-collision theory, and its applications to nuclear reactions, atomic physics, and molecular structure. He has published widely on these topics, has lectured and done research in many countries, has edited/co-edited several research compilations, is the founder/first chairman of the American Physical Society's Topical Group on Few-Body Systems and Multi-particle Dynamics, is an awardee of the Alexander-von-Humboldt-Stiftung, and is a Fellow of the American Physical Society. Among the large variety of courses he has taught are the year-long graduate and undergraduate courses on quantum mechanics at Brown University. The present text is an outgrowth of these teaching experiences.

Preface

Quantum mechanics, the theoretical framework that describes microscopic physical phenomena, is a marvelous intellectual enterprise. Elegant, intriguing, challenging, often counter-intuitive and sprinkled with delightful surprises, it is wholly unlike classical physics. Mastery of quantum theory is an essential ingredient in the education of physicists and chemists. This text, a broad and deep introduction to the theory, is intended not only to help provide that mastery but also to convey to the reader its inherent richness.

The book is designed for use in year-long undergraduate courses, for self-study, and as a supplemental text in graduate courses. Its aims are achieved through a combination of introductory material, including a survey of relevant mathematics; an axiomatic formulation of the theory via six postulates; applications to soluble one-, two-, and three-dimensional systems; theoretical augmentations such as symmetry properties, electromagnetic interactions, spin $\frac{1}{2}$ and generalized angular momentum; and discussion of approximation methods and their application to electromagnetic transitions and systems of identical fermions (atoms and molecules). The reader is assumed to be familiar with material covered in courses on intermediate mechanics, electromagnetism and elementary modern physics, plus mathematics through vector calculus, elements of partial differential equations (their form and separation-of-variables solutions), and some linear algebra (finite dimensions, matrices).

The writing of this book has been strongly influenced by the author's experiences teaching both the graduate and the undergraduate quantum-theory courses at Brown University. Most of the students who take the undergraduate course are junior-level physics majors, many of whom go on to graduate school in physics. Like that undergraduate course, this text is intended to provide a solid preparation for graduate courses on quantum theory. In doing so, it also stresses the fact that quantum mechanics is an evolving subject in which new and sometimes surprising developments have occurred and old controversies have been reinvigorated. Indeed, the second half of the twentieth century has seen developments in quantum mechanics undreamed of in its first 25 years of existence. Among those discussed in this book are various phase effects (Aharonov–Bohm, Berry, etc.); hidden-variable analysis (Bohm, Bell, etc.); identification of a system-dependent, quantal time operator; Feynman's path-integral formulation; and coherent states. Discussions of other sublime topics include exponential time decay, time–energy uncertainty relations, spin regeneration, gauge invariance, minimal coupling, classical limits, scattering of spin-$\frac{1}{2}$ projectiles, fine- and hyperfine-structure effects in hydrogen, and Hartree–Fock theory for atoms.

The book is substantial. This is partly a result of the author's belief that a quantum-mechanics textbook should contain thorough explanations and partly a result of his desire to treat a wide variety of topics in a reasonably full fashion. Since this has led to expanded discussions, one chapter and a number of sections and subsections have been starred: they can be omitted without seriously compromising the pedagogical development. Even with such omissions, however, there is still more material than can be covered in a year-long course. The book contains essentially all the topics the author would include in a course for which the usual academic time constraints could be ignored. Since these constraints cannot be ignored, instructors who adopt this text will be able to select from a wide-ranging menu of possible subjects against which they can structure a course.

Veteran teachers of quantum theory will know how tempting it is to continue a specific analysis beyond what is needed for an adequate treatment of most topics. While some of these additional analyses are presented, the author has tried to avoid undue excess in this regard, choosing instead to cite references that the interested reader may consult. The text is peppered with references to a variety of other material, including many of the original articles on particular topics. This should help to restore to the contemporary scene the names of possibly forgotten scientists whose results were not only the first published but were also inspiring to others.

Analyses involving electromagnetic quantities occur in various places in the text, especially Chapter 12. Although SI units have been adopted universally and are standard in almost all undergraduate books on electromagnetism, cgs units are still found in some widely adopted graduate-level quantum-mechanics texts. Anyone who will read or encounter one of these texts (e.g., those by Baym and by Sakurai) should be familiar with cgs as well as SI units. Consequently, in this book electromagnetic quantities are expressed in terms of constants whose values in both sets of units are explicitly stated. For example, the Coulomb interaction between charges q_1 and q_2 separated by a distance r is written $\kappa_e q_1 q_2/r$, where $\kappa_e = 1/(4\pi\varepsilon_0)$ in SI units and $\kappa_e = 1$ in cgs units, with the q's defined appropriately.

In addition to this particular piece of pedagogy, the author has indulged in another conceit: the use of a variety of acronyms, examples being w.r.t. for "with respect to"; LHS and RHS for "left-" and "right-hand side"; 1-D, 2-D, and 3-D for "one," "two," and "three dimensions," respectively; the usual abbreviations viz., i.e., and e.g.; etc. For the author their felicity overcomes any lack of grace their use may entail. Correspondingly, the adjective "quantal" is used not only to replace the less-felicitous phrase "quantum-mechanical," but also as a sharp reminder that the subject matter is not "classical." From this viewpoint, "quantal" and "classical" can be considered as "Through the Looking Glass" mirror images.

Although the organization of this book is stated in its table of contents, details and specific items can be discovered only by reading the text. For the newcomer to quantum mechanics who wishes to learn the theory through self-study, the author's advice is to start with Chapter 1 and read sequentially, possibly ignoring all portions set off with an asterisk. All readers should work through the exercises: they are intended as learning tools. Some extend and enrich theoretical concepts, others flesh out various applications; few are of the "plug-in" variety. Some of the exercises contain hints on how to proceed, whereas in others there is a statement of the result to be derived. Instructors should note that not all parts of a long exercise need be assigned.

An instructor who uses this book as a primary text will be melding his/her teaching background and preferences with the material and its presentation. In addition to there being too many topics to fit into a two-semester course, the level of the students obviously needs to be taken into account. Depending on where in the physics curriculum an undergraduate course on quantum theory occurs and what the components of that curriculum are (e.g., a previous modern-physics course or mathematics courses on linear algebra) the first semester could cover topics from the first ten chapters, although it is probably more likely that Chapters 1–7 plus 9 will comprise the first semester.

In structuring a course around this text (or simply when reading it), it may be helpful to know some of the author's intentions concerning the chapters and specific material they contain. For example, in addition to its historical and review aspects, Chapter 1 is designed to start the reader thinking in quantal terms: its exercises dealing with orders of magnitude are especially important here. Chapter 2 continues along the path of thinking quantally. For very-well-prepared students, the topics of these first two chapters could be touched on lightly in lectures, with most of the material assigned for independent reading.

There are many ways of arranging a first meeting with quantum mechanics. The one adopted in Chapter 3, which compares the classical stretched string and the 1-D quantal box, also includes a brief review of waves. Eigenvalue problems are first encountered in this chapter. They are presented in the context of differential equations – which are presumed to be familiar to readers – rather than via matrices. The omittable Section 3.4 introduces the important concepts of Hermiticity and the Dirac delta function, still in the context of differential equations (and Sturm–Liouville systems). These concepts occur again in Chapter 4, where the notions of abstract operators and their matrix realizations are exemplified by the 3-D rotation operator/matrix, which is assumed to be familiar from a course in classical mechanics. Chapter 4 is included to help make the book self-contained, especially if it is used as the text in a junior-year course. Most of this chapter is a not-very-rigorous survey, and much of it will be a review for fourth-year students who have already taken a course on mathematical methods, in which case the instructor can make a selection of topics for lectures and assign the rest as independent reading.

Since this book's approach is axiomatic, the formal theory is presented in Chapter 5 via six postulates. The postulates are illustrated using 1-D (one-degree-of-freedom) systems in Chapters 6 (bound states) and 7 (continuum states). The multiple approaches to the linear harmonic oscillator in Chapter 6 allow an instructor great latitude in dealing with this system: the author's preference is to discuss all of them. Continuum states are the subject of a separate chapter because their Hilbert-space (normalizable, wave-packet) nature is an aspect that, in the author's opinion, needs to be stressed more than the 1-D character of the system. The plane-wave limit is straightforward and the continuum examples then treated are standard. However, by going through the 1-D wave-packet analysis, the stage is set for its 3-D analog in Chapter 15.

How much, if any, of Chapter 8 will be touched on will depend on time constraints and an instructor's taste. While this chapter is omittable, Chapter 9 is NOT: it contains essential theoretical developments. It, along with Chapter 5, is the foundation on which the rest of the text is built. Especially important here are the sections on complete sets of commuting operators and symmetry operations.

With Chapter 10, one enters the 3-D, core portion of undergraduate courses on quantum mechanics. The coordinate-space approach to orbital angular momentum and its eigenvalue problem is deliberate: by postponing the algebraic method to Chapter 14, one focuses in this chapter on the angular dependence, the connection between the $\ell(\ell+1)\hbar^2$ eigenvalue and convergence (discussed in Appendix C), the relationship between ∇^2 and $\hat{L}^2$, etc. Sections 10.3 and 10.4 may be considered as examples illustrating orbital angular momentum.

In one sense, Chapter 11 contains additional examples of orbital angular momentum. However, these are incidental to its real purpose, viz., to introduce the reader to "realistic" if not real problems, ranging from the treatment of a two-body system as an equivalent one-body system to the discussions of accidental degeneracies. As with the linear oscillator of Chapter 6, the differential equation for the attractive $1/r$ potential is solved and discussed in detail.

Because the quantal treatment of external, classical electromagnetic fields is a subject of great elegance, it deserves a chapter to itself. That elegance, especially made manifest through gauge invariance and the Aharonov–Bohm effect, is discussed in detail in Chapter 12, but, for the time-constrained instructor, its first three sections should suffice. Electromagnetic fields are treated before intrinsic spin. Hence, prior to reading about the Stern–Gerlach experiment, one has learned that, when a spinless particle in a spherically symmetric potential is acted on by a constant (weak) magnetic field, each of its energy levels is split into an odd number of components. The stage is thus set for the spin-$\frac{1}{2}$ interpretation of the Stern–Gerlach experiment, which is discussed in Section 13.1.

The nature of spin $\frac{1}{2}$ makes it one of the most sublime constituents of the quantum treasury, and the analysis in Chapter 13 strives to convey this assessment. That spin $\frac{1}{2}$ is a two-state system helps to substantiate this, as does the solving of the eigenvalue problem for an arbitrary quantization direction. Additional ingredients that the author finds particularly appealing are the direct experimental basis on which two graduate students (!!) constructed their theoretical framework, and the regeneration of extinguished spin components.

Generalized angular momentum need not be included in an undergraduate quantum-mechanics course. However, it and the developments associated with it that are treated in Chapter 14 are crucial elements in this text. Because of this, an instructor who plans to cover the later material in this book dealing with dipole transitions, fine- and/or hyperfine-structure effects in hydrogen, the Pauli principle and two-electron atoms as well as atomic-spectroscopic term values, will need to cover Sections 14.1 and 14.3. Once Section 14.1 has been included, it would be very difficult (at least for the author) to resist including Section 14.2. The final section, on Bell's inequality, is intended for independent study.

It is not unusual to find scattering theory either omitted or treated near the end of undergraduate quantum-mechanics texts. However, since scattering states are the continuum states in 3-D, and Part III is largely concerned with 3-D, for the author it is a logical necessity to include scattering theory in Part III. It is also a logical necessity to begin Chapter 15 with a wave-packet analysis, since only a wave packet can be a proper quantum state in the continuum.

Part IV of this book introduces the reader to some of the approximate procedures for dealing with realistic as well as real systems. The order in which certain material occurs in Part IV is unusual; in particular, time-dependent perturbation theory (Chapter 16) occurs before its time-independent counterpart (Chapter 17). This ordering is based on the author's belief that related topics should be treated as close together as possible. Since electromagnetic fields and the Aharonov–Bohm effect are considered in Chapter 12, time-dependent processes such as electromagnetic transitions and those related to geometric phases are discussed as soon as is feasible, viz., in Chapter 16. Of course, whether either or both of these topics will be included in a course is the instructor's decision. The author's hope is that some of the various geometric-phase material can be touched on, since studies and measurements of quantum phases are an intrinsic part of the physics developed during the latter half of the twentieth century.

Chapter 17 treats most of the standard time-independent approximation methods. Section 17.2 is a beautiful application of perturbation theory to the model H-atom of Chapter 11, and it may well be worth making time for this analysis. On the other hand, the analysis of Section 17.4 cannot be omitted if any of Sections 18.2, 18.4, and 18.5 is to be studied. Section 18.1 is essential: a physicist's undergraduate education is incomplete if it has not included some material on identical-particle symmetries. As for the rest of Chapter 18, an instructor has much to choose from for lectures, and much to assign as possible independent reading. An example is the wide-ranging discussion of approximate calculations on He: the intent here is to show the reader the degrees of accuracy and the quality of the associated physical pictures resulting from simple to highly sophisticated computations.

The selection and organization of the material that forms this book is the author's sole responsibility. Nevertheless he has benefited from, and usually incorporated, the suggestions of various colleagues regarding improvements. In this regard he is indebted to Antal Jevicki, to Janine Shertzer, to the anonymous reviewers, and to Stavros Fallieros, who also made his extensive collection of homework problems available for use in this text. It has taken many years to finish this book, the writing of which has occurred in various locales, on the water as well as on land. The author is grateful to the many marinas and harbors where safe havens and stable environments were provided to CHEERS, on whose chart table a good deal of the writing has taken place. The jocular encouragement of sailing friends, especially Eric and Daisy Broudy and David and Barbara Constance, has been a helpful reminder that even as serious an undertaking as writing a book on quantum mechanics is still a playful activity. The first typing of almost all of the text was done by Winnie Isom, whose role in the preparation of this text has been enormous: she has earned the author's thanks many times over. Additional kudos in this regard go to Nadine Catteral and Elizabeth Peña and to Etta Johnson and Chantée Watts. It is an additional pleasure to acknowledge the splendid support provided by past and present members of the Cambridge University Press community: Simon Capelin, Jo Clegg, Steve Holt, Zoe Naylor, Eoin O'Sullivan, Sue Tuck, and especially Phil Meyler, who convinced his colleagues to take a chance on the author's mammoth text. Finally, and most important of all, this book could not have been written without the unfailing love, patience, and support of the author's wife, Carol Levin, to whom it is dedicated.

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Part I

INTRODUCTORY

1

The Need for a Non-Classical Description of Microscopic Phenomena

Quantum mechanics is the theoretical framework that describes physical phenomena on the microscopic scale. In particular, it is used in those situations in which Planck's constant h, approximately equal to 6.62×10^{-34} J s, cannot be assumed to be negligible, despite its apparently tiny magnitude. Macroscopic phenomena, on the other hand, involve magnitudes that are so large that h can be set equal to zero without appreciable error.

As an illustration of this in the macroscopic context, consider the following example: a ladybug (*Hippodamia convergens*) of mass 1 g moves radially at a speed of 0.01 m s^{-1} on a turntable rotating at 10 rpm. In the rotating frame of reference, the ladybug has a kinetic energy of about an erg, and, in the laboratory frame, its angular momentum is roughly 10^{-5} J s when it is at a distance of 0.1 m from the center of the rotating turntable. The latter angular momentum is of the order of $10^{28} h$. Thus, relative to this value, h is well approximated by zero and, indeed, only classical mechanics is needed to describe the ladybug's motion.

In contrast to the preceding example, an electron in the "2p" level of hydrogen has an energy of about 10^{-25} J and an angular momentum whose magnitude is approximately $h/(2\pi) \equiv \hbar$ (pronounced "h-bar"). Here, h cannot be ignored and only a quantum description can accurately account for the properties of this system.

The latter example cites the 2p energy level of the H-atom. One of the goals of this book is to show how quantum mechanics describes the hydrogen atom. This particular "how" involves an understanding both of the postulates of quantum theory and of various technical/mathematical details, topics that are examined beginning in Chapter 5 on the quantal postulates. However, "how" is not the only question that can be raised. Another is "why?" Why is quantum mechanics necessary, i.e., what is the compelling evidence that a non-classical description of microscopic phenomena is needed? This first chapter is concerned with that necessity.

Quantum theory was developed mainly during the first thirty years of the twentieth century. In retrospect, its development can be considered a direct consequence of three key concepts that classical physics has never been able to explain. These are (i), the particle nature of electromagnetic radiation, i.e., the existence of light quanta or photons; (ii), the quantization of energy and of angular momentum; and (iii), the wave nature of particles. Each concept was introduced in order to explain experimental data and each has been verified countless times. All three have major theoretical implications. These concepts are examined in detail in the following subsections via experiments and data