Quantum Mechanics

Designed for a two-semester advanced undergraduate or graduate-level course, this distinctive and modern textbook provides students with the physical intuition and mathematical skills to tackle even complex problems in quantum mechanics with ease and fluency. Beginning with a detailed introduction to quantum states and Dirac notation, the book then develops the overarching theoretical framework of quantum mechanics, before explaining physical quantum-mechanical properties such as angular momentum and spin. Symmetries and groups in quantum mechanics, important components of current research, are covered at length. The second part of the text focuses on applications, and includes a detailed chapter on quantum entanglement, one of the most exciting modern applications of quantum mechanics, and of key importance in quantum information and computation. Numerous exercises are interspersed throughout the text, expanding upon key concepts and further developing students' understanding. A fully worked solutions manual and lecture slides are available for instructors.

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‘Berera and Del Debbio do a wonderful job of walking the reader through the mathematics of quantum theory, never shying away from the necessary complexities while keeping things as simple as they can be.’

David Tong, University of Cambridge

‘Today’s quantum mechanics students should learn not only the harmonic oscillator and the hydrogen atom, but also entanglement and quantum information. This book treats the old and the new with great clarity, including a first look at quantum computation through the Deutsch and Grover algorithms. Another highlight is the collection of well-crafted problems.’

Matthew Reece, Harvard University

‘This text promises to be useful to a wide audience, from intermediate-level undergraduates to beginning graduate students. It is pedagogical and rather complete, and attempts to guide readers with different backgrounds via gentle yet precise mathematical asides. The chapter on quantum entanglement is the most comprehensive and complete discussion of the topic in a broad quantum mechanics textbook and will play an important role in introducing twenty-first-century undergraduates to the contemporary and rapidly growing field of quantum computing.’

André de Gouvêa, Northwestern University

‘Quantum mechanics is difficult to teach as it defies intuitions of everyday experience. The textbook by Berera and Del Debbio grounds the subject by laying its mathematical foundations first, giving students a coherent framework distilled from a century of teaching experience. Filled with helpful exercises and modern topics including quantum information theory, this book would be an excellent text for both undergraduate and graduate courses.’

Maxim Lavrentovich, University of Tennessee, Knoxville

‘One of the best features of this book is the substantial chapter on quantum entanglement, quantum computing and information theory (Bell’s inequality, no-cloning theorem, quantum teleportation). It is based on early introduction of the mathematical foundations and Dirac notation. Beyond the standard topics, students will appreciate the inclusion of symmetry groups, applications involving multi-electron systems, the WKB(J) method, the discussion of the Dirac equation, and an in-depth treatment of quantum scattering.’

Russell Herman, University of North Carolina

‘A concise yet complete introduction to quantum mechanics at the undergraduate level. The authors do a great job of exploring the formal and qualitative aspects of the theory, as well as more modern topics of interest such as quantum computation.’

Christopher Aubin, Fordham University

‘Arjun Berera and Luigi Del Debbio’s *Quantum Mechanics* is an exceptional textbook. It, of course, offers superb coverage of the requisite material for a standard two-semester upper-level undergraduate quantum mechanics (QM) course. Nonetheless, the textbook is much richer than that. Two features make it unique: Chapter 1, “Stories and Thoughts about Quantum Mechanics”, presents a detailed and lively history of “the tortuous path that led to the formation of the theory as we know it”. This reading both is entertaining and sets the groundwork for the chapters that follow. Also of special note is Chapter 15, “Quantum Entanglement”. While quantum entanglement has long raised theoretical questions regarding freedom and the nature of reality, within the last two decades its applications have burst forth not just in physics, but also in engineering, computing, encryption and communications. Through very informative chapter readings and well-chosen problems, students will master associated key concepts, such as calculating and interpreting Bell's inequality; information theory and Shannon and von Neumann entropies; the no-cloning theorem, quantum teleportation and superdense coding; and quantum register and logic gates, Deutsch's algorithm and Grover's algorithm. This textbook sets the standard for quantum entanglement coverage. I ardently promote Arjun Berera and Luigi Del Debbio's *Quantum Mechanics*.'

Gerald B. Cleaver, Baylor University

'Lucid introduction to a complex subject accessible to advanced undergraduate and beginning graduate students in science and engineering. The authors combine physical insight and mathematical rigour in explaining abstract concepts with a variety of examples. Covers all the quintessential topics in the field, as well as a valuable modern introduction to quantum entanglement.'

Kaladi Babu, Oklahoma State University

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For our parents

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Preface

Quantum mechanics is one of the most successful scientific theories ever developed and is responsible for the vast majority of modern technology including computers and smartphones, lasers and telecommunications and magnetic resonance imaging. In its most basic form, quantum mechanics tells us that at the microscopic level, matter can behave both as a particle and as a wave. Such a simple concept leads to a fundamental shift in our understanding of how the world works.

The identification of mathematical physics as a distinct discipline at the University of Edinburgh can be traced back to 1922. Since then, notable physicists such as Charles Galton Darwin, Max Born, Nick Kemmer and Peter Higgs (to mention a few) have taught this programme, and contributed not only to its high-quality teaching but also to developing and updating course lecture notes. Today, as the current custodians of the quantum mechanics course, we have taken this accumulated knowledge of teaching this course and turned it into this textbook, whose key features are:

1. The inclusion of key, modern chapters on symmetries in quantum mechanics and quantum entanglement, as well as an extensive chapter on scattering.
2. The introduction of Dirac notations from the beginning to explain complex equations.
3. The adoption of a modern approach to introducing quantum mechanics via the mathematical underpinnings (Hilbert spaces, linear operators, etc.).
4. Detailed in-text examples and numerous end-of-chapter problems, which will enable students to better understand and practise the concepts discussed.

The market for this textbook is intermediate and senior undergraduate physics students. We appreciate that students' mathematical background can vary and so we have deliberately chosen to discuss these topics without assuming any previous subject knowledge. The goal is simply to enable the reader to acquire the basic principles that are covered in each chapter and be able to do basic calculations. Admittedly, some sections are treated in more detail than others, making them appeal also to graduate students and researchers. For instance, the time-independent perturbation theory chapter covers both higher-order perturbations and second-order degenerate perturbation theory. For time-dependent perturbation theory the first-order results are analysed in detail and the formal expressions at higher orders are derived. In the WKBJ section, a full treatment utilising this approximation is given for the double well; and in the quantum scattering chapter, a derivation of scattering starting with a wave packet is carried out, showing the reader how that can then be replaced by a plane wave state. The units throughout the book are Gaussian (cgs).

Overall though, this textbook encompasses all the standard topics covered in a one-year course. This now also includes an extensive chapter on quantum entanglement, which is becoming a standard topic needed within a quantum mechanics course. Instructors will also be able to access online a set of lecture slides and a solution manual to all the end-of-chapter problems.

Book Organisation

- **Chapter 1: Stories and Thoughts about Quantum Mechanics.** This is an introductory chapter, which summarises the historical development of quantum mechanics. It can be read in isolation as a source of trivia on the early days of the discipline. It also gives the reader an idea of the tortuous path that led to the formulation of the theory as we know it. In the rest of the book we have decided to opt for a systematic treatment of quantum mechanics, where the principles are stated from the very beginning and their consequences are then analysed, without spending too much time discussing how these principles emerged. We believe that this approach makes it easier for the reader to understand the logical framework of quantum mechanics. This first chapter is a necessary reminder of the fact that revolutionary ideas in physics are the result of a long process of trial and error, during which theoretical ideas are compared and challenged by experimental results and vice versa.
- **Chapter 2: Quantum States.** This chapter lays the foundation of our description of the states of a quantum system as vectors in complex vector spaces. We decided to introduce complex vectors, and Dirac's notation, from the very beginning since they provide the correct mathematical framework to discuss quantum mechanics. We aim to provide a self-consistent presentation, with mathematical details presented in separate *Mathematical Asides*. We study in detail the case of *two-state systems* and *one-dimensional quantum systems*. The first is a simple example of a vector space of quantum states, which is actually relevant in the description of numerous physical systems. The latter explains the connection between the description of quantum states using vectors and the one using wave functions.
- **Chapter 3: Observables.** The second ingredient that is needed in order to set up a theory of quantum phenomena is the concept of observables. Observables in quantum mechanics are treated in a peculiar and very precisely defined manner. Here we use the word 'peculiar' to emphasise the difference from the intuitive idea of an observable that we have from our everyday experience and from classical mechanics. In particular, this chapter introduces the probabilistic nature of measurements in quantum mechanics and discusses the far-reaching consequences of it. When discussing a quantum-mechanical experiment we need to adhere strictly to the postulates of the theory that specify what can be predicted about the outcome of these experiments. A central role is played by Hermitian operators acting in the vector space of physical states. These new concepts are illustrated in this chapter, together with the mathematical tools that are necessary for their implementation. As in the previous chapter, we aim to give sufficient mathematical details so that the reader can follow all the manipulations that are discussed.

- **Chapter 4: Dynamics.** This chapter presents the postulates that define the time evolution of a quantum state, i.e. the changes of the state vectors as a function of time. The time evolution is dictated by Schrödinger's equation, where the Hamiltonian (i.e. the operator associated with the energy of the system) determines the change of the state vector during an infinitesimal amount of time. We present a generic method to solve for the time evolution of a system once the Hamiltonian is known, and then focus on the time evolution of the wave function for a one-dimensional system. We present some general properties of the solution of Schrödinger's equation in a one-dimensional potential.
- **Chapter 5: Potentials.** Building on the material presented in Chapter 4, this chapter is devoted to the solution of the Schrödinger equation for a number of simple potentials. These are good examples, which can be solved explicitly, and provide some insight on the dynamics of quantum systems. The emphasis in this chapter is on two aspects. First, the technical solution of the equations that appear in the examples. These are typical manipulations that the reader needs to become familiar with and therefore we provide a fair amount of detailed discussion. Second, once we have the solution of the equations, we need to learn how to extract their physical interpretation, according to the principles that were laid out in the early chapters. Both aspects are important and need to be 'digested' by the reader. Exercises and problems are designed to build and consolidate the mathematical tools needed.
- **Chapter 6: Harmonic Oscillator.** The harmonic oscillator plays a central role in physics, since every potential close to its minimum can be approximated by a quadratic potential. This chapter presents the quantum-mechanical treatment of a system that evolves in a harmonic potential. We set up the Schrödinger equation for this system and present its solution using both algebraic methods and a *brute force* solution of the second-order differential equation. The algebraic solution allows us to introduce creation and annihilation operators, which are important concepts that are used in many applications.
- **Chapter 7: Systems in Three Spatial Dimensions.** This chapter presents the generalisation of concepts that were already discussed in previous chapters to the case of systems in three-dimensional space. While this is a crucial step for the description of most quantum systems in nature, going from one-dimensional to three-dimensional space is a straightforward procedure, which allows us to revise some of the material that has already been encountered. In particular, we discuss again the relation between complex vectors and wave functions. We discuss a new technique, known as separation of variables, and apply it to study the harmonic oscillator in three dimensions. We also see for the first time an explicit example of degenerate eigenvalues.
- **Chapter 8: Angular Momentum.** Angular momentum plays a central role in describing the properties of a quantum state under rotations. In this chapter we introduce a Hermitian operator that we associate with the orbital momentum of a quantum system and study its properties. We compute the commutation relations that characterise the Cartesian components of angular momentum, and express the corresponding operators as differential operators acting on the wave function. We identify a set of compatible observables and search for their common eigenstates. We find that angular momentum

is quantised, and compute the corresponding eigenfunctions. All the basic features of angular momentum are introduced in this chapter, which is a prerequisite for the following four chapters.

- **Chapter 9: Spin.** This chapter introduces the concept of intrinsic angular momentum, i.e. a type of angular momentum that is not related to the spatial dependence of the wave function. This intrinsic angular momentum is known as *spin* and is a peculiar property of quantum mechanics. We summarise the properties that spin shares with the orbital angular momentum introduced in the previous chapter, and then focus on spin's peculiarities. We discuss in detail the properties of spin-$\frac{1}{2}$ systems that are relevant to discuss the elementary constituents of matter like the electrons.
- **Chapter 10: Addition of Angular Momenta.** In this brief chapter we explain the rules for adding angular momenta in quantum mechanics. These are useful when considering the total angular momentum of a system that is made up of multiple subsystems, or when adding the orbital angular momentum and the spin of a particle. We keep this chapter short, focusing on giving a set of practical rules, rather than aiming at deriving them. This chapter is the final part of the discussion of angular momentum that we started in Chapters 8 and 9.
- **Chapter 11: Central Potentials.** Central potentials are characterised by the fact that they only depend on the distance from the origin. As such, they describe the dynamics of systems that are symmetric under rotations in three spatial dimensions. Working in spherical coordinates it is possible to reduce the Schrödinger equation for these systems to a one-dimensional problem for the radial dependence of the wave function. Building on our previous discussion of orbital angular momentum, this chapter presents in full detail the mathematical steps that lead to the one-dimensional formulation of the problem. These methods are general and applicable to any radial potential. The chapter includes the study of the quantum rotator and the central square well as examples of central potentials. The content of this chapter is an essential prerequisite for the discussion of the hydrogen atom.
- **Chapter 12: Hydrogen Atom.** Pulling together all the tools that have been introduced so far in the book, we are in a position to discuss the energy levels of the hydrogen atom. This is one of the great successes of quantum mechanics, solving one of the problems that had exposed the limits of validity of classical physics. Once again, the emphasis is on presenting the detailed calculation so that the reader can follow the derivations step-by-step and check their understanding of the basic principles. A physical interpretation of the mathematical results is presented at the end of the chapter.
- **Chapter 13: Identical Particles.** Because quantum mechanics does not allow us to define the 'trajectory' of a particle – we cannot have states that are localised in one point in space with a given momentum because of the Heisenberg uncertainty principle – identical particles need to be treated as indistinguishable entities. The mathematical translation of this statement is that the state vector is unchanged (more precisely, only changes by a phase factor) under a permutation of the two particles. This seemingly logical statement has deep consequences, which are summarised in the spin-statistics theorem and the Pauli exclusion principle.

- **Chapter 14: Symmetries in Quantum Mechanics.** Symmetries play a central role in our description of natural phenomena. In this chapter we define the concept of symmetry transformations in both classical and quantum mechanics, and discuss how the set of symmetry transformations of a physical system naturally forms a mathematical structure called a *group*. We discuss in detail two important examples, namely the group of translations and the group of rotations. We introduce the *generators* of these groups and identify them with the operators respectively associated with momentum and angular momentum. We conclude the chapter with a discussion of the general properties of the set of generators, showing that it has the structure of an algebra. Even though we do not have the opportunity to fully develop the mathematical formalism in this book, the reader should get an idea of some of the fundamental underlying ideas, which have shaped the contemporary understanding of physical phenomena.
- **Chapter 15: Quantum Entanglement.** One of the challenges in writing this book has been including a textbook-level chapter on quantum entanglement. This is a growing subject area not only in physics but also in engineering, computing and communication, and one that physics students taking quantum mechanics should have a sound understanding of.

  This chapter presents a modern account of quantum entanglement and is aimed at all physics undergraduates in their intermediate years and requires no previous knowledge of the subject. The chapter has select topics, which all combined provide the reader with a solid foundation yet can be covered within a few weeks. The chapter fits seamlessly with the other more traditional topics in quantum mechanics presented in the book. Of course, we do appreciate that some of the more mathematical aspects that the chapter includes might be better suited for advanced undergraduate physics students or graduate students. However, the goal is making sure that – once the reader has completed this chapter – they will know the key concepts and be able to do basic calculations relevant to the subject.

  The *main topics* covered are the Einstein–Podolsky–Rosen (EPR) paradox, Bell's inequality, quantum teleportation, quantum computing, including the Deutsch and Grover algorithms. We also introduce quantum information theory, including a brief background to Shannon entropy and classical information theory, followed by a discussion of von Neumann entropy and entanglement entropy. For those interested in knowing more about this subject, the literature included in the References and Further Reading sections at the end of the chapter offers some good tips. Note also that since the topics discussed in this chapter are still evolving and emerged relatively recently compared to other topics in quantum mechanics, we have cited as footnotes some of the key seminal papers. This is the only chapter where some original journal articles are cited.
- **Chapter 16: Time-Independent Perturbation Theory.** This is one of the most well-used approximation methods in quantum mechanics. There is a derivation of nondegenerate perturbation theory, done up to third order in the energy correction. In addition, the normalisation and orthogonality of the eigenstates is done up to second order. Degenerate perturbation theory is then derived and developed up to second order in the energy correction. Application of perturbation theory to hydrogen fine structure is treated along

with an Appendix that derives these fine-structure terms from the relativistic Dirac theory. The first-order perturbation theory correction to the ground-state energy of helium is also treated.

- **Chapter 17: Calculation Methods Beyond Perturbation Theory.** The Rayleigh–Ritz variational method is presented for estimating the ground-state energy of a system. The first excited state of the helium atom is treated by perturbation theory followed by a broader discussion for treating multi-electron atoms. The Born–Oppenheimer approximation is discussed. This method is useful for problems where there are heavy and light masses in a system. An application of this method is given for the hydrogen molecular ion. The Hellmann–Feynman method is given, which takes derivatives of the Hamiltonian operator with respect to some judiciously chosen parameters to extract results on expectation values of the system. Finally, the Wenzel–Kramers–Brillouin–Jeffreys (WKBJ) approximation is addressed for treating problems where the potential is slowly varying relative to the variation of the wave function. The WKBJ treatment of the potential well and barrier, as well as the symmetric double well, are presented in detail.
- **Chapter 18: Time-Dependent Perturbation Theory.** In this chapter, we examine problems where the Hamiltonian depends on time. The formalism of time-dependent perturbation theory is developed as an approximation method to compute transitions between a specified set of basis states. The general first-order expression is given and specific examples are given of a constant perturbation switched on at some given time and a harmonic perturbation. Interaction of radiation with a quantum system is treated at the lowest non-trivial dipole approximation. Absorption, stimulated emission and spontaneous emission of photons by a quantum system are considered, and the Einstein coefficients are obtained. Selection rules based on symmetry considerations are derived. The time-dependent perturbation theory formalism is derived to all orders.
- **Chapter 19: Quantum Scattering Theory.** The scattering of a particle with a potential is examined. Expressions for the scattering amplitude and *scattering cross-section* are derived for the lowest-order Born approximation and the Born series. The scattering of a wave-packet is treated to understand how it can then be replaced by a plane wave. Partial wave analysis, useful for low-energy scattering, is treated as a complementary method to the Born series, which is most useful at high energy.

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Alongside some of our own approaches, the lectures over the years have absorbed and modified what our programme has considered the best explanations from other classic textbooks on quantum mechanics, including Bransden and Joachain, Cohen-Tannoudji, Gasiorowicz, Griffiths, Landau and Lifshitz, Liboff, Merzbacher, Messiah, Sakurai, Schiff, Shankar, and many others.

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