Preface: Who Can Benefit from Reading This Book?

Nanoscience and nano-engineering are rapidly growing fields that break the boundaries between classical disciplines such as Physics, Chemistry, Biology, and Engineering. The potential for utilizing nanoscale devices in very different applications, including, for example, medicine, electronics, or information and data processing, drives research efforts toward unraveling the way nature works on the nanoscale. One thing that immediately becomes apparent is that the rules of Quantum Mechanics (QM) are necessary for understanding nature on this scale. In fact, it was the development of experimental techniques with nanoscale resolution that revealed the wave–particle duality and contributed to the formulation of QM in the early twentieth century (for example, the X-ray crystallography contributed to the discovery of the wave nature of electrons in the Davisson–Germer experiment, discussed in Chapter 1).

Along with the potential for advancement and the growing interest in nanoscience and nano-engineering comes the challenge of making the principles of QM accessible and useful to researchers from different fields. Scientists and engineers turning to nanotechnology from diverse disciplines such as biology, chemical engineering, or mechanical engineering often lack formal education in QM, and sometimes lack even the mathematical experience or technical skills needed to learn QM from a standard introductory textbook. Moreover, the research in nanoscience and engineering is motivated by "real-world" problems that require rather advanced topics not usually addressed in introductory textbooks. For example, most textbooks would address the exact solution of the Schrödinger equation for an isolated hydrogen atom, but not the "real-world" phenomena of electron tunneling into an atom on a surface, or electron transfer between impurities in a condensed phase environment. While the mathematics needed to describe (at least approximately) the latter phenomenon is less cumbersome in comparison to the analytic solution of the hydrogen atom problem, advanced applications are excluded from introductory textbooks since they require the introduction of advanced QM topics relevant to open quantum systems (Chapters 17–19) or nonequilibrium states (Chapter 20).

In this book we propose a pedagogical approach aimed at making advanced QM theory accessible for readers interested in QM and its applications in general, for researchers entering the fields of nanoscience and engineering, as well as for deep thinkers who wish to master the field. Three features make our approach unique and different from standard approaches to teaching QM. The first feature is the close relation to "real-world" phenomena and applications from nanoscience and technology, which often motivate the theoretical discussions and/or summarize each topic. In many of the chapters, the study of the theory will be motivated by problems from the realm of nanotechnology, mapping them onto fundamental questions and answering these questions via acquaintance with the principles of QM. The manifestation of the postulates and the mathematical structure of the theory in experimental observations will be emphasized. The second feature is the inclusion of advanced topics (commonly met in applications to “real-world” problems) within an introductory-level textbook. The third feature is the “layered” structure of the text, which should be appealing to both “rigorous” and “easy” readers. For the benefit of the latter, the reading is kept relatively fluent by defining the most technical details and mathematical proofs as exercises appearing next to the main text. Some of the exercises are standard, but most of them are guided instructions for proving equations or justifying claims made in the main text. Just reading these guided exercises may be convincing enough for some of the more technically oriented readers, while the most rigorous readers would probably want to actively succeed in solving the exercises, thus gaining a complete hold on any claim and equation mentioned in the book.

It is emphasized that the postulates and the mathematical structure of nonrelativistic QM are presented at a fairly rigorous level, along with mathematical technicalities required, for example, for solution of ordinary differential equations or dealing with tensor product spaces. In this sense, the book can also serve the more rigorous readers who wish to master the field, including undergraduate and graduate Physics students.

In Chapter 1 we introduce the reader to the necessity for using QM to understand phenomena on the nanoscale, where the wave–particle duality naturally appears. This chapter leads to a basic introduction to wave functions and probability densities (Chapter 2), observables as operators (Chapter 3), and the Schrödinger equation (Chapter 4). While discussing the solutions of the stationary Schrödinger equation for different model systems in the following chapters (Chapters 5–10), we emphasize relations to applications in nanotechnology. For example, the ability to control the observed color (light absorption or emission) associated with nanoparticles of different size is relevant in numerous applications. This phenomenon motivates our fundamental discussion of energy quantization in QM in Chapter 5. Indeed, relating “color” to energy level spacing, we provide a rigorous discussion of energy quantization and of the “quantum size effect.” Similarly, the discussion of experimental methods for characterization of nanoscale objects, such as Scanning Tunneling Microscopy (STM), motivates our theoretical discussion of the quantum tunneling phenomena, first for bound particles (quantum wells) (Chapter 6), and then for free particles (quantum barriers) (Chapter 7). The latter motivates the introduction of theoretical concepts such as probability current density and the first encounter with quantum scattering theory. The investigation of mechanical motions in nanoscale systems by infrared and microwave spectroscopies motivates our introduction to quantization of vibrations and rotations in many-atom systems (molecules, solids) and to the fundamental models of the quantum harmonic oscillator and the quantum rigid rotor in Chapters 8–9. In Chapter 10 we address the structure of atoms as the building blocks of matter on the nanoscale by starting from the solution of the Schrödinger equation for the single-electron (hydrogen like) atom. After extensive exposure to solutions of the Schrödinger equation for simple systems in Chapters 5–10, the mathematical formulation and the postulates of QM are rigorously given in Chapter 11. To establish a basis for the more advanced discussions, approximation methods based on perturbation theory and on the variation principle are introduced in Chapter 12. The variation of electronic properties between different elements (the periodic table) motivates our discussion of the electronic structure of many-electron atoms in Chapter 13, within the mean-field (orbital) approximation. In Chapter 14 the structure of many-atom systems is addressed in molecules and in periodic crystals, where the nature of chemical bonds is analyzed. The relation between the chemical composition of a material and its electric conductivity is thus also revealed. The more advanced themes start with a rigorous introduction to quantum dynamics in Chapter 15 and proceed to quantum thermodynamic systems (mixed ensembles) in Chapter 16. Elementary rate processes in nanoscale systems are most relevant for "real-world" applications such as photovoltaic cells or electro-optical devices. Their study motivates our discussion of transport processes and quantum kinetics. In Chapter 17 the emergence of unidirectional rate processes in QM is introduced within the framework of time-dependent perturbation theory, where Fermi's golden rule for the rate constant is derived. Applications to processes such as light absorption and emission, charge, and energy (exciton) transfer between impurities in bulk materials and between molecules in solution are discussed in Chapter 18. In Chapter 19 we address the dynamics in open quantum systems, the validity of the Markovian approximation, and the emergence of irreversible dynamics and relaxation to equilibrium. Chapter 20 provides the theoretical basis needed for the description of quantum charge transport in nanoscale devices under nonequilibrium conditions, motivated by the applications of molecular electronic devices.

In conclusion, this book exposes the reader to the foundations of quantum mechanics, to the richness of quantum phenomena on the nanoscale, and to the theoretical understanding of the physics underlying these phenomena. The reader gains a solid basis in the theory of nonrelativistic QM, its fundamental postulates, and its practical implementation. The book provides the language and the concepts needed for addressing more specified QM texts such as advanced textbooks and research articles dealing with nanoscale phenomena and their applications. Moreover, the reading and the active learning associated with solving the many guided exercises in this book aim to provide our readers also with skills that should enhance their own creativity in addressing "real-world" problems encountered on the nanoscale.