Book & Media Reviews

Introduction to Quantum Mechanics: in Chemistry, Material Science, and Biology

by S. M. Blinder

Elsevier Academic Press: Amsterdam, 2004. 319 pp.
ISBN 0121060519 (paper). $47.95

reviewed by Kevin M. Dunn

What part of modern chemistry is more counterintuitive, more maddeningly complex, more difficult to explain to the novice, or more fundamental to the science than quantum mechanics? In general chemistry it provides the foundation for the periodic table. In organic chemistry it forms the basis for understanding structure, bonding, and reactivity. Yet it is in undergraduate physical chemistry that the naked mathematical underpinnings of quantum mechanics are first exposed in all of their bewildering glory. In *Introduction to Quantum Mechanics* S. M. Blinder, professor emeritus at the University of Michigan, lays out the machinery of quantum mechanics for the advanced undergraduate or beginning graduate student. The book is intended as a "less weighty" text for one semester of physical chemistry or for a stand-alone course. While pitched to students of chemistry, it would be of interest to those in materials science, molecular biology, earth sciences, and physics, as well. In addition to the material commonly covered in a college-level introduction, Blinder has included a thorough discussion of metaphysical questions that dominate literature for the lay public but which are generally slighted in college textbooks.

Introduction to Quantum Mechanics is laid out along traditional lines, beginning with a discussion of the failures of classical physics at the beginning of the twentieth century. Indeed, with notable exceptions, the chapters fall in the same order and at roughly the same level of difficulty as those in most introductory physical chemistry textbooks. Chapter Two uses the double-slit experiment to motivate the introduction of operators and eigenvalues. While most physical-chemistry textbooks begin with the particle in a box, Chapter Three begins with the free particle, introducing the notion of superposition at the earliest natural opportunity. The particle-in-a-box adds boundary conditions to the free particle, resulting in integral quantum numbers and discreet energy levels. Once we have the solution to this simple problem, it is immediately applied to the free-electron model for delocalized π electrons, providing a relevant example of chemical interest. The generalization of the particle in a box to three dimensions introduces the notion of degeneracy. With these examples at hand, Chapter Four lays out the postulates of quantum mechanics and applies the variational principle to the particle in a box.

Chapters Five through Eight work through the harmonic oscillator, rigid rotor, hydrogen atom, and helium atom. Just as the particle in the box was applied to conjugated polyenes, the particle on a ring is applied to aromatic molecules, providing a chemically-relevant example. The level of these three chapters is midway between the typical graduate and undergraduate texts. For example, while ladder operators are used in the solution of the harmonic oscillator, as is commonly done in graduate texts, they are not used for the rigid rotor. Rather, the spherical harmonics are simply presented as solutions to the relevant differential equation, as is commonly done in undergraduate texts. Spin is introduced as a special case of rotation and the Pauli spin matrices appear in a supplement. As with angular momentum, the solutions to the hydrogen atom are presented in the chapter and explored in more depth in a supplement. The helium atom is solved variationally and its ground and excited states are briefly explored before moving on to general n-electron wavefunctions.

Chapter Nine applies the principles of the previous chapters to the general atomic problem, though it does not go much beyond the typical general-chemistry text in discussing atomic states. While term symbols are introduced, they are always for the ground state of the atom. Spin-orbit coupling is not discussed at all and so no mention is made that a single electron configuration can give rise to several electronic states. In particular, while the ground state terms are worked out for the first row of the periodic table, the low-lying excited states of carbon and oxygen are not mentioned. This would have been an ideal place to reflect on the spin-orbit splitting of atomic spectra, mentioned in Section 6.6. As it is, however, the neglect of the excited electronic state at this stage prevents a more thorough discussion of electronic spectroscopy later in the book.

Chapter Ten reviews fundamentals of chemical bonding, including the Heitler–London solution for the hydrogen molecule, valence bond theory, hybrid orbitals, VSEPR, and crystal field theory. The quantum mechanical treatment of bonding appears in earnest with the solution of the hydrogen molecule ion in Chapter Eleven. LCAO–MO theory is used to generalize to polyatomic molecules. Term symbols are used to describe the ground states of simple homonuclear diatomic molecules and ions, though as with the atoms, excited states are not discussed. Chapter Twelve applies the quantum mechanics of the previous chapters to chemically-relevant examples. Hückel Theory is introduced along with the Woodward–Hoffmann rules. Band theory is used to describe conductivity in metals and semiconductors and the principle of the diode, transistor, and LED are developed in some detail. The Hartree–Fock and density-functional methods are introduced and the student is directed to free computer programs for making these calculations.

The remaining chapters, with one notable exception, follow the order typical of undergraduate physical-chemistry texts. Group theory appears in Chapter Thirteen with immediate application to the molecular orbitals of the ammonia and water molecules. Chapter Fourteen develops vibrational, rotational, and electronic spectroscopy of diatomic and polyatomic molecules. Chapter Fifteen is devoted to NMR, including pulsed techniques, Fourier transforms, and 2-D

NMR. This concludes the material usually included in undergraduate physical chemistry. Professor Blinder, however, has left the best for last.

Books on quantum mechanics fall into two broad classes. First, there are books written by non-scientists for non-scientists, focusing on those metaphysical, counterintuitive aspects of quantum mechanics which so often provide the *deus ex machina* for science-fiction novels, explorations of artificial intelligence, and how-to guides for expanding one's consciousness to cosmic dimensions. Second, there are books by scientists for scientists, focusing on the potentially-dry mathematical bones upon which the meatier metaphysical interpretations hang. The final chapter of *Introduction to Quantum Mechanics* places it into a third, virtually unpopulated class of books. Having developed the mathematical foundations of quantum mechanics, Professor Blinder turns to metaphysical concerns that are generally shrouded in jargon and analogy by authors who might or might not be able to take the derivative of the exponential function. Here Blinder devotes an entire chapter to material which receives only a paragraph or two at the hands of most textbook authors. The Copenhagen interpretation, Schrödinger's ill-fated cat, superposition and entanglement, Bell's theorem and Aspect's experiment, teleportation and quantum computing, all rest comfortably on the mathematical foundation laid down in earlier chapters. Unlike many students weaned on three-inch-thick textbooks, readers of *Introduction to Quantum Mechanics* may be able to compute expectation values for the harmonic oscillator *and* hold their own at cocktail parties, though not necessarily at the same time.

Physical-chemistry textbooks generally top a thousand pages these days, in part because authors and publishers must include every topic whose elimination might offend a significant fraction of the faculty market. Professor Blinder has shaved a hundred and fifty pages off of the quantum-mechanical content of the typical undergraduate textbook resulting in a volume which is one-third as thick and half the cost. Coupled with introductory books on thermodynamics and kinetics, it could be used to teach undergraduate physical chemistry, as suggested in the preface to the book. The chosen thermodynamics book, in particular, would need to address statistical thermodynamics, which is beyond the scope of this book. A professor looking to be offended by missing content would probably be disappointed by the minimal attention given to the excited electronic state. Another might complain that most chapters provide fewer than ten end-of-chapter problems. A graduate chemistry professor might find that the level of the text seldom goes beyond that of undergraduate physical chemistry. For these reasons, *Introduction to Quantum Mechanics* is probably best suited as a graduate text for students outside chemistry who need to understand quantum mechanics without undertaking a full year of physical chemistry. In addition to mastering the *mechanics,* lucky readers of this book will explore the fascinating philosophical and metaphysical implications that launched into popular culture the word, *quantum.*

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