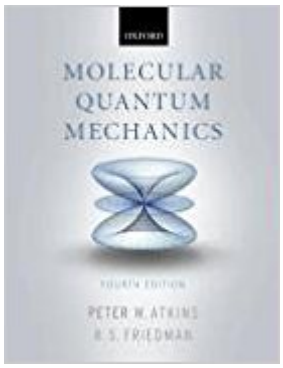
Molecular Quantum Mechanics



Synopsis

Quantum mechanics embraces the behaviour of all known forms of matter, including the atoms and molecules from which we, and all living organisms, are composed. Molecular Quantum Mechanics leads us through this absorbing yet challenging subject, unravelling those fundamental physical principles which explain how all matter behaves. With the clarity of exposition and rich pedagogy which have established the book as a leading text in the field, Molecular Quantum Mechanics takes us from the foundations of quantum mechanics, through quantum models of atomic, molecular, and electronic structure, and on to discussions of spectroscopy, and the electronic and magnetic properties of molecules. Lucid explanations and illuminating artworks help to visualise the many abstract concepts upon which the subject is built. Fully updated to reflect the latest advances in computational techniques, and enhanced with more mathematical support and worked examples than ever before, Molecular Quantum Mechanics remains the ultimate resource for those wishing to master this important subject. Supplementary resources Companion web site, featuring: Illustrations available to download Solutions manual available to download [instructors only]

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Customer Reviews

`Review from previous edition 'Undoubtedly amongst the best textbooks of quantum mechanics at this level'' Endeavour``a remarkable tour de force'' Journal of Chemical Education``beautifully produced, clearly and attractively written, and contains a wealth of worked examples and problems for classroom use'' Times Higher Education Supplement``This is a precious classic, carefully

adapted to the needs of modern readers.'' Paul Popelier, Chemistry and Industry, July 2005

Professor Peter W. Atkins, Professor of Chemistry, and Fellow of Lincoln College, University of Oxford, UK Dr Ronald S. Friedman, Professor, Department of Chemistry, Indiana University Purdue University Fort Wayne, USA

I have been reading reviews in this forum about this book. A few reviewers compare this book with two other popular quantum chemistry textbooks, namely, McQuarrieÃƒÂ¢Ã â ¬Ã â„¢s ÃƒÂ¢Ã â ¬Ã Å“Quantum ChemistryÃƒÂ¢Ã â ¬Ã Â• and LevineÃƒÂ¢Ã â ¬Ã â„¢s ÃƒÂ¢Ã â ¬Ã Å“Quantum Chemistry. I do not think it is an apple-to-apple comparison. First McQuarrieÃƒÂ¢Ã â ¬Ã â„¢s book is only an entry-level book. All the mathematical derivations are clearly laid out. There are hardly any doubts that McQuarrie's exposition of the subject is much better. For students that are mathematically less inclined and want to learn quantum chemistry, McQuarrieÃƒÂ¢Ã â ¬Ã â„¢s book is the best among the three. However, only topics that are considered as traditional training for a chemist are covered in McQuarrie's book. After all the preliminaries such as particle in a box, operators, simple harmonic oscillator, angular momenta and perturbation theory, the book focuses on electronic theories of atoms and molecules. Both McQuarrie's and Atkins' books use the method of creation and annihilation operators to solve the Schrodinger Equation for a simple harmonic oscillation. Levine's book still uses the traditional power series method. Mathematically, the operator method is definitely much more elegant. LevineÃƒÂ¢Ã â ¬Ã â„¢s book is very similar to McQuarrieÃƒÂ¢Ã â ¬Ã â„¢s book; mathematically it is on a much higher level. Both books hardly touch on group theory.Mathematically, AtkinsÃƒÂ¢Ã â ¬Ã â„¢ book is more compact and advanced than McQuarrieÃƒÂ¢Ã â ¬Ã â„¢s book. Unlike McQuarrieÃƒÂ¢Ã â ¬Ã â„¢s book, the mathematical derivations are not laid out in a step-by-step fashion. In principle, a person who has well working knowledge of calculus should have no problems with the mathematics. All other necessary mathematics are presented at the end of each chapter. To better understand this book, it is important to follow the mathematics with a pencil and a piece of paper. Mathematical techniques such as gradient, Laplacian, curl and divergence of a vector field, matrices, complex numbers, Dirac delta function, ordinary and partial differential equations are frequently used.AtkinsÃƒÂ¢Ã â ¬Ã â„¢ book covers a wide range of topics in quantum mechanics. These include group theory, optical activity, electric properties of molecules, magnetic properties of molecules and scattering theory. These topics are generally not covered in a few quantum chemistry texts. Although it has a chapter on computational chemistry, its

coverage is less extensive than that of LevineÃƒÂ¢Ã â ¬Ã â„¢s. Levine's book devotes 4 chapters on molecular modeling (one chapter is on electron correlation). The chapter on group theory is fairly extensive and it includes proofs of the Great and Little Orthogonality Theorems, the constructions of character tables, projection operators and rotational groups. This chapter provides all the most common techniques that are used in chemistry. The last two chapters are probably the most sophisticated ones. It introduces concepts such as vector potential, gauge transformation and invariance, central potential. scattering amplitude and scattering phase shift. Of all the quantum chemistry and NMR books that I have read, this is the only book I come across that shows the full derivation of the Lamb formula, the diamagnetic contribution to shielding in NMR spectroscopy. Although integral equation and GreenÃƒÂ¢Ã â ¬Ã â„¢s function are used in the last chapter on scattering theory, a person with a good background of calculus should not have any difficulties in understanding mathematics in the Born approximation.If you are interested in the mathematics of quantum physics, this is a book for you. Since it is a book on molecular quantum mechanics, it does not cover topics such as spin, identical particles, density matrices, quantum computing (e.g. quantum encryption) and foundations of quantum mechanics (e.g. hidden variables and Bell Inequality). All these topics can be found in David MillerÃƒÂ¢Ã â ¬Ã â„¢s book, ÃƒÂ¢Ã â ¬Ã Å“Introduction to Quantum Mechanics to Scientists and EngineersÃƒÂ¢Ã â ¬Ã Â•. Mathematically, MillerÃƒÂ¢Ã â ¬Ã â„¢s book is on the same level, may be slightly lower, as that of AtkinsÃƒÂ¢Ã â ¬Ã â„¢ book. These two books do not presume knowledge of advanced classical mechanics such as Hamiltonian and Lagrangians. Miller's book makes a fine compliment to Atkins' book.If you have mastered McQuarrieÃƒÂ¢Ã â ¬Ã â„¢s and LevineÃƒÂ¢Ã â ¬Ã â„¢s books, I think you should have a copy this book. The mathematics and quantum mechanics in AtkinsÃƒÂ¢Ã â ¬Ã â„¢ book are really interesting. It is worth spending the time to understand the mathematics.

I have always thought that Atkins' textbooks were horrible. His worst book was Physical Chemistry, only the 2nd edition was good, then it deteriorated considerably (now I think it's up to the 8th edition! very hard to read that book). This one, Molecular Quantum Mechanics, has an excellent selection of topics, and is mostly a book that will teach you about spectroscopy techniques for the study of molecules (NMR, ESR, vibrational spectroscopy, rotational spectroscopy, etc). It does a fairly good job at teaching things with minimal assumed background. So anyone with basic calculus and some intro to QM should be able to read this book. Atkins derives much of the QM tools needed for the rest of the book (e.g. time-dependent perturbation theory). His presentation of the more

"mathematical" topics is generally very lucid. With the exception of the section on group theory, which I've always thought was incomprehensible. You will find a MUCH better (and friendly) learning tool in D.C. Harris' (dover) book. Group theory is taught without any nonsense. I also like Bernath's textbook for group theory (that's about the only thing that's good in Bernath). Anyhow, Atkins IS a good buy. You will learn a lot from it, and it can serve as an excellent supplement to any course on quantum mechanics. He is very pedagogical, and the book includes tons of relevant worked examples. Many of them are non-trivial too, so it makes you feel good, that you've learned new stuff and improved your skills. I would say this is a good book, from an author who usually writes mediocre textbooks.

Buy McQuarrie and Simon's "Physical Chemistry" or Griffith's "Introduction to Quantum Mechanics" instead of this book. The book is too concise, and it skips a considerable amount of math. The math is awkwardly addressed in his Mathematical Background and Further Information chapters. Also, the book is, overall, harder to understand. It may be the way the way the author words the sentences or the notation he uses for equations. I have spent hours trying to decipher what the author was trying to say in several chapters. I felt cheated on the time that I had to spent on this book to understand the concepts it illustrated.

I used this text after struggling for the first few weeks in my quantum chemistry course at Berkeley. Recommended by my professor, this text made sense of things that I believed impossible. And, it includes a lot of graphs to boot! I found this book coupled with Griffith's Quantum Mechanics to have been the best possible undergrad combo in my junior year as a chemistry undergrad. In fact, I sold my required text and passed the class with flying colors using just the Atkins book and the Griffith text. Where Atkins is too wordy, Griffith's concise explanations help greatly. And, vice versa, when you need more info, turn to Atkins. Bon chance!

Very good book with good explanations of different topics. If only I had learned quantum mechanics from this textbook, I would be better off.

Being four chapters into this textbook now, and with a decent background in mathematics, I feel very strongly that this book has set a bar for explanation of difficult phenomena. At no point does the ideas presented seem unreachable, and the build from topic to topic is masterful. Sincerely, I am glad to be using this text for this subject.

This book is the best quantum chemistry book. All issues are clear and didatic. I recommend, mainly because the frist chapters explains the postulates like no other book.

Used this book for a graduate quantum class. Atkins, despite having written several books in physical chemistry, is useless. This is a very basic textbook with several notation errors. Oxford books: find a physicist that will write a clear and descriptive quantum textbook for use across multiple disciplines.

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