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Robert L. Brooks

The Fundamentals of Atomic and Molecular Physics

Springer

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Preface

This book represents an expansion of a set of course notes for a fourth year undergraduate course in atomic and molecular physics. It assumes two semesters of quantum mechanics as background and could just as easily be called an applied quantum mechanics text. It presents material central to an understanding of structure for both atoms and molecules, developed with a thoroughness not seen in texts since the classics of John C. Slater. It makes no attempt to cover scattering or the multitude of modern topics related to trapping, cooling, or condensation. When used for a 12 week course at the senior undergraduate level, a term paper on some modern topic of the student's interest has been assigned as a supplement and together offer an excellent grounding for students interested in graduate work, whether in this area or some other. Indeed, most of the students taking this course have gone on to study other areas of physics.

The quantum mechanics of complex atoms is not easy to grasp when only cursory or simplified explanations are offered. There seems to be some tacit assumption among authors that only quantum chemists need to know this material and so it is given short shrift in most texts when treated at all. The frustrating thing for many students is that graduate work often assumes that they know this material and yet it is developed from the basics in no book at this level. Whereas many texts develop the two-electron atom using techniques that are not applicable to the many-electron atom, this one treats the two-electron atom as the simplest example of the multi-electron atom and then turns to carbon, as an example, without needing to develop additional equations.

Perturbation techniques are then used to treat fine-structure, the Zeeman and Stark effects, and hyperfine structure. Complications that arise from intermediate coupling or from external fields are handled by direct diagonalization and, for fine structure, are then compared with the results from first-order perturbation.

Spontaneous emission from an atom or molecule in an excited state is another fundamental process which is not often developed from the foundations of time-dependent perturbation theory through the expression for the lifetime of the excited state. Advanced texts can start with Fermi's golden rule while quantum mechanics texts often end there. Developing these expressions in detail is good pedagogy for the student. Asking the question, why does an excited atom decay at all, can stimulate the student to learn quantum electrodynamics even as the answer can be understood, though incompletely, without that.

The electronic structure of diatomic molecules is not so easily accessible as the ro-vibrational interactions and so most books will start with the latter. But if one has just completed a study of the electronic structure of atoms, then to start with the electronic structure of the simplest molecule, $H_2{}^+$, makes a lot of sense. Prolate spheroidal coordinates are used, which are natural to the problem, and afford the student usually the first example of performing quantum mechanics using coordinates other than Cartesian, cylindrical, or spherical. The student can perform all of the needed integrals. After that the H_2 molecule is taken up which becomes the molecular analogue of progressing from the hydrogen atom (one electron system) to the complex atom (multi-electron system). One cannot overstate the usefulness, toward understanding molecular bonding, of solving the quantum mechanics of the hydrogen molecular ion and molecule. The ro-vibrational excitations of diatomic molecules are taken up in the final chapter in sufficient detail to satisfy the needs of those progressing toward further study as well as for those not likely to see this material in graduate school.

For most of the years that this material has been used for a fourth year elective course at the University of Guelph it has attracted between 10 and 20 students with the latest numbers nearing thirty. The overwhelming majority of students have gone on to other areas of physics and many have returned to say that this course was where they learned quantum mechanics. I can think of no higher praise.

Guelph, ON, Canada Robert L. Brooks

Acknowledgements

Turning my lecture notes into a textbook started when one of my students, Theo Hopman, took it upon himself to type up my handwritten notes in LaTeX format. But the first serious suggestion and real impetus for this project was made by Gordon Drake and I am grateful to both of them. Dennis Tokaryk has used the original notes for a number of years and provided invaluable feedback. More than a nod of appreciation should go to my editors Jace Harker and HoYing Fan at Springer. Finally, thanks to the dozens of students who have pointed out typos, mistakes, and confusions whose resolution has greatly improved the final text.

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