
Preface

Atomic, Molecular and Optical physics – short **AMO** physics – is one of the canonical fields of physics, a profound knowledge of which is essential for understanding almost any other area of modern physics. And while its roots reach back over a century and are closely connected with the early days of modern physics, current research in **AMO** physics is still highly productive in respect of both, cutting edge applications and fundamental insights – as several NOBEL prizes in recent years have documented convincingly.

Looking back at the technical development of modern industrial society – which is closely connected with modern physics – one may refer (COSE, 1998) to the 20th century as that of the electron while the 21st is the century of the photon. This interesting particle, the essential ingredient of modern optics and quantum optics, surprises humankind since NEWTON with its wave-particle dualism. It does not only play a key role in today's information technology but is, from a general point of view, also the primary carrier of any information which can be obtained about the constituents of matter and materials. Even collisions of particles with mass under the influence of the COULOMB force may be viewed as exchange of virtual photons.

The textbooks presented here try to give a fairly comprehensive overview on the whole field. They cover state of the art experimental methods, and combine this with preparing the basis for a serious, theory based understanding of key aspects in modern **AMO** research. The two volumes, originally written in German language (HERTEL and SCHULZ, 2008), are a genuine authors translation – not just an English mirror image of the original. We have rewritten much of the text, extended it wherever appropriate, and updated a number of aspects to catch up with recent progress in the field.

On the one hand we address advanced students of physics, chemistry and other neighbouring fields, typically at the end of their undergraduate studies, or during their doctoral work. On the other hand we also wish to reach young postdocs or even mature scientists, who feel it is time they connect freshly with the topics addressed here. We consider the basics of classical geometrical optics and wave optics as well as electrodynamics to be well known by our readers. We also expect a cer-

tain basic knowledge and understanding of atomistic concepts in physics, as well as of elementary quantum mechanics.

We do, however, provide in Chaps. 1 and 2 of this Vol. 1 a brief repetition of these topics – essentially an extended list of keywords focussed on basic understanding and knowledge. In the main part we cover the standard scope of atomic physics, touch some modern aspects of spectroscopy, and try to lead the reader up to state-of-the-art research in some main areas of the field – wherever possible and as far as space permits. The sequence of chapters follows essentially the logics of perturbation theory. The strongest perturbation is treated first. Thus, after the introductory chapters where pure COULOMB interaction and the H atom have been discussed, in Chap. 3 we allow for coarse deviations from the $1/r$ potential and focus on quasi-one-electron systems. This, and some common sense, allows us already to introduce the periodic system of elements. Next, in Chap. 4, we have to treat optically induced and spontaneous transitions: they are a central theme in AMO physics. This requires a brief introduction to time dependent perturbation theory, a topic which is indispensable in AMO physics, but which is often neglected in undergraduate quantum mechanics. To allow the reader a step by step approach towards the more demanding topics, we implement at this point ‘only’ the semiclassical approach – by which 95 % of standard atomic physics may be treated (resorting occasionally to somewhat hand waving arguments) – and postpone field quantization to Vol. 2.

Chapter 5 further extends this knowledge, treating shapes and widths of spectral lines and introducing multiphoton processes as well as transitions into the continuum. We are now ready to understand in Chap. 6 a next step of complication, fine structure (FS) interaction. In order to allow the reader to appreciate the experimental efforts, we also give a brief introduction to high resolution and precision laser spectroscopy. This leads us automatically to the LAMB shift and calls for a short side step into the basics of quantum electrodynamics (QED). In Chap. 7 two electron systems are treated, mainly the He atom and He like ions. Exchange interaction may be smaller or larger than FS, depending on the system, but the step to multielectron systems adds a new degree of complexity and sets the stage for a quantitative treatment of the PAULI exclusion principle.

The next finer step in the hierarchy of perturbations is treated in Chap. 8, including interactions between atomic electrons and external magnetic and electric fields, leading to ZEEMAN and STARK effect, respectively. At this point, a small detour into the world of interaction between atoms and very intense laser fields is appropriate, as the theoretical formalism used is essentially an extension of the so called *dynamical STARK effect*. As a last refinement we include in Chap. 9 hyperfine interactions between the atomic nucleus and electrons. These lead to very small but highly significant splittings of atomic energy levels (HFS) and offer a wealth of practical applications. In the last Chap. 10 of Vol. 1 we are finally ready to treat genuine multi-electron systems with a large number of electrons. We discuss the appropriate theoretical tools (such as HF equations, CI methods, and DFT), and present some relevant methods of X-ray spectroscopy and sources for generating X-ray radiation.

As a rule, we try to avoid extensive mathematical derivations. Rather, in the ‘spirit of these books’ we prefer to give the reader some general guidance on how to reach

the final, physically important results – which we discuss and illustrate usually in some detail. In addition, we provide several appendices for the reader interested in more detail. We have e.g. collected a toolbox for angular momentum algebra in atomic and molecular physics – without any claim for full mathematical consistency, but quite compact and possibly useful in practice.

Some words about formats, notation, units, typography appear in order:

- Each chapter begins with a brief “*motto*” setting the tune of the chapter, followed by short abstract guiding the reader through the text. At the end of each section a short summary recalls what the readers should have learned from the preceding text. All chapters build upon each other, but may be read by advanced readers also individually: this is facilitated by intensive cross referencing of formulas and figures, extended indices covering both volumes, a list of acronyms and important terminology as well as references at the end of each chapter.
- For clarity and homogeneity we do not reproduce original drawings or other material from the literature. Rather, all published data have been redrawn (after digitalization if necessary), are presented in a standard format, and all sources used in the figures and text are properly quoted.
- We consequently use the SI-System for all measurable quantities, and we emphasize the pedagogical and practical value of a “dimensional analysis” for complex physical formulas.¹ On the other hand, atomic units (a.u.) facilitate the writing of many relations in atomic and molecular physics dramatically. Hence, we use them intensively – considering, however, E_h , a_0 and t_0 etc. simply as abbreviations for quantities with dimensions. Phrasings such as “we set \hbar , e , m_e , c equal to unity” are avoided, since they are highly misleading.
- The finite number of letters in the Latin and Greek alphabets makes some inconsistencies or unusual designations unavoidable: we mention specifically, that in order to allow the use of E for the electric field strength (an important quantity in AMO) we use W (with appropriate indices) for energies of various types (with the exception of the atomic unit of energy which is internationally defined as E_h). Occasionally we use the letter T for kinetic energy and try to avoid the neighbourhood of time and temperature which are often also designated by T . Vectors are written as \mathbf{r} or \mathbf{k} , unit vectors in these directions are \mathbf{e}_r and \mathbf{e}_k , respectively. We write operators as \hat{H} , vector-operators as $\hat{\mathbf{p}}$ and tensors of rank k as \mathbf{C}_k . For the unit operator and unit matrix we use $\hat{\mathbf{1}}$. For integer numbers we mostly use calligraphic letters such as \mathcal{N} , while number densities are simply N to distinguish them from the index of refraction n which is also an often used quantity throughout this text. Oscillations and other periodic processes are mostly characterized by their angular frequencies ω (sometimes also by their frequencies ν) and the corresponding energies are $\hbar\omega$ (or $h\nu$).

¹We make, however, use of allowed prefixes (NIST, 2000a), such as cm^{-1} as unit of wavenumbers (which appears ineradicable in the literature). We also use “accepted” units outside the SI (NIST, 2000b), such as the enormously practical energy unit eV (electronvolt), or b (barn) as unit for cross sections.

Finally, we hope that these books will become a continuing source of reference for the fastidious reader, working in or just needing to use **AMO** physics in her or his special field. We ask all of you to kindly provide us with the necessary feedback. We shall try to react to useful suggestion promptly. At the home page of the books, <http://www.mbi-berlin.de/AMO/book-homepage>, we shall continuously report on the status, list errata and possibly present additions. For additional reading and cross referencing we have collected a few related textbooks and monographs in the reference list below, just as typical examples without any claim for completeness.

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January 2014

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Acronyms and Terminology

AMO: ‘Atomic, molecular and optical’, physics.

a.u.: ‘atomic units’, see Sect. 2.6.2.

CI: ‘Configuration interaction’, mixing of states with different electronic configurations in atomic and molecular structure calculations, using linear superposition of SLATER determinants (see Sect. 10.2.3).

DFT: ‘Density functional theory’, today one of the standard methods for computing atomic and molecular electron densities and energies (see Sect. 10.3).

FS: ‘Fine structure’, splitting of atomic and molecular energy levels due to spin orbit interaction and other relativistic effects (Chap. 6).

HF: ‘HARTREE-FOCK’, method (approximation) for solving a multi-electron SCHRÖDINGER equation, including exchange interaction.

HFS: ‘Hyperfine structure’, splitting of atomic and molecular energy levels due to interactions of the active electron with the atomic nucleus (Chap. 9).

NIST: ‘National institute of standards and technology’, located at Gaithersburg (MD) and Boulder (CO), USA. <http://www.nist.gov/index.html>.

QED: ‘Quantum electrodynamics’, combines quantum theory with classical electrodynamics and special relativity. It gives a complete description of light-matter interaction.

References

- ATKINS, P. W. and R. S. FRIEDMAN: 2010. *Molecular Quantum Mechanics*. Oxford: Oxford University Press, 2nd edn.
- BERGMANN, L. and C. SCHAEFER: 1997. *Constituents of Matter – Atoms, Molecules, Nuclei and Particles*. Berlin, New York: Walter der Gruyter, 902 pages.
- BLUM, K.: 2012. *Density Matrix Theory and Applications*. Atomic, Optical, and Plasma Physics 64. Berlin, Heidelberg: Springer Verlag, 3rd edn., 343 pages.
- BORN, M. and E. WOLF: 2006. *Principles of Optics*. Cambridge University Press, 7th (expanded) edn.

- BRANDSEN, B. H. and C. J. JOACHAIN: 2003. *The Physics of Atoms and Molecules*. Prentice Hall Professional.
- BRINK, D. M. and G. R. SATCHLER: 1994. *Angular Momentum*. Oxford: Oxford University Press, 3rd edn., 182 pages.
- COSE (Committee Optical Science and Engineering): 1998. *Harnessing Light: Optical Science and Engineering for the 21st Century*. Washington, D.C: National Academy Press, 360 pages.
- DEMTRÖDER, W.: 2010. *Atoms, Molecules and Photons*. Berlin, Heidelberg, New York: Springer, 2nd edn.
- DRAKE, G. W. F., ed.: 2006. *Handbook of Atomic, Molecular and Optical Physics*. Heidelberg, New York: Springer.
- EDMONDS, A. R.: 1996. *Angular Momentum in Quantum Mechanics*. Princeton, NJ, USA: Princeton University Press, 154 pages.
- HERTEL, I. V. and C. P. SCHULZ: 2008. *Atome, Moleküle und optische Physik 1; Atomphysik und Grundlagen der Spektroskopie*. Springer-Lehrbuch. Berlin, Heidelberg: Springer-Verlag, 1st edn., 511 pages.
- HERTEL, I. V. and C. P. SCHULZ: 2010. *Atome, Moleküle und optische Physik 2; Moleküle und Photonen - Spektroskopie und Streuphysik*, vol. 2 of *Springer-Lehrbuch*. Berlin, Heidelberg: Springer-Verlag, 1st edn., 639 pages.
- NIST: 2000a. 'Reference on constants, units, and uncertainties: SI prefixes', NIST. <http://physics.nist.gov/cuu/Units/prefixes.html>, accessed: 8 Jan 2014.
- NIST: 2000b. 'Reference on constants, units, and uncertainties: Units outside the SI', NIST. <http://physics.nist.gov/cuu/Units/outside.html>, accessed: 8 Jan 2014.
- STEINFELD, J. I.: 2005. *Molecules and Radiation, An Introduction to Modern Molecular Spectroscopy*. Mineola, NY: Dover Edition, 2nd edn.
- WEISSBLUTH, M.: 1978. *Atoms and Molecules*. Student Edition. New York, London, Toronto, Sydney, San Francisco: Academic Press, 713 pages.



<http://www.springer.com/978-3-642-54321-0>

Atoms, Molecules and Optical Physics 1

Atoms and Spectroscopy

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2015, XXXVII, 689 p. 285 illus., 265 illus. in color.,

Hardcover

ISBN: 978-3-642-54321-0