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Springer Handbook
of Atomic, Molecular, and Optical Physics

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Foreword by Herbert Walther

The Handbook of Atomic, Molecular and Optical (AMO) Physics gives an in-depth survey of the present status of this field of physics. It is an extended version of the first issue to which new and emerging fields have been added. The selection of topics thus traces the recent historic development of AMO physics. The book gives students, scientists, engineers, and other interested people a comprehensive introduction and overview. It combines introductory explanations with descriptions of phenomena, discussions of results achieved, and gives a useful selection of references to allow more detailed studies, making the handbook very suitable as a desktop reference.

AMO physics is an important and basic field of physics. It provided the essential impulse leading to the development of modern physics at the beginning of the last century. We have to remember that at that time not every physicist believed in the existence of atoms and molecules. It was due to Albert Einstein, whose work we commemorate this year with the world year of physics, that this view changed. It was Einstein's microscopic view of molecular motion that led to a way of calculating Avogadro's number and the size of molecules by studying their motion. This work was the basis of his PhD thesis submitted to the University of Zurich in July 1905 and after publication became Einstein's most quoted paper. Furthermore, combining kinetic theory and classical thermodynamics led him to the conclusion that the displacement of a microparticle in Brownian motion varies as the square root of time. The experimental demonstration of this law by Jean Perrin three years later finally afforded striking proof that atoms and molecules are a reality. The energy quantum postulated by Einstein in order to explain the photoelectric effect was the basis for the subsequently initiated development of quantum physics, leading to a revolution in physics and many new applications in science and technology.

Prof. Dr. Herbert Walther

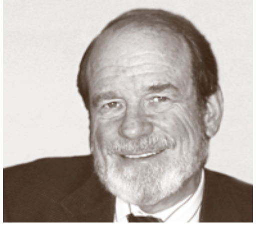
The results of AMO physics initiated the development of quantum mechanics and quantum electrodynamics and as a consequence led to a better understanding of the structure of atoms and molecules and their respective interaction with radiation and to the attainment of unprecedented accuracy. AMO physics also influenced the development in other fields of physics, chemistry, astronomy, and biology. It is an astonishing fact that AMO physics constantly went through periods where new phenomena were found, giving rise to an enormous revival of this area. Examples are the maser and laser and their many applications, leading to a better understanding of the basics and the detection of new phenomena, and new possibilities such as laser cooling of atoms, squeezing, and other nonlinear behaviour. Recently, coherent interference effects allowed slow or fast light to be produced. Finally, the achievement of Bose–Einstein condensation in dilute media has opened up a wide range of new phenomena for study. Special quantum phenomena are leading to new applications for transmission of information and for computing. Control of photon emission through specially designed cavities allows controlled and deterministic generation of photons opening the way for a secure information transfer.

Further new possibilities are emerging, such as the techniques for producing attosecond laser pulses and laser pulses with known and controlled phase relation between the envelope and carrier wave, allowing synthesis of even shorter pulses in a controlled manner. Furthermore, laser pulses may soon be available that are sufficiently intense to allow polarization of the vacuum field. Another interesting development is the generation of artificial atoms, e.g., quantum dots, opening a field where nanotechnology meets atomic physics. It is thus evident that AMO physics is still going strong and will also provide new and interesting opportunities and results in the future.

Preface

The year 2005 has been officially declared by the United Nations to be the International Year of Physics to commemorate the three famous papers of Einstein published in 1905. It is a fitting tribute to the impact of his work that the *Springer Handbook of Atomic, Molecular, and Optical Physics* should be published in coincidence with this event. Virtually all of AMO Physics rests on the foundations established by Einstein in 1905 (including a fourth paper on relativity and his thesis) and his subsequent work. In addition to the theory of relativity, for which he is best known, Einstein ushered in the era of quantum mechanics with his explanation of the photoelectric effect, and he demonstrated the influence of molecular collisions with his explanation of Brownian motion. He also laid the theoretical foundations for all of laser physics with his discovery (in 1917) of the necessity of the process of stimulated emission, and his discussions of the Einstein–Podolsky–Rosen Gedanken experiment (in 1935) led, through Bell's inequalities, to current work on entangled states and quantum information. The past century has been a Golden Age for physics in every sense of the term.

Despite this history of unparalleled progress, the field of AMO Physics continues to advance more rapidly than ever. At the time of publication of an earlier Handbook published by AIP Press in 1996 I wrote "The ever increasing power and versatility of lasers continues to open up new areas for study." Since then, two Nobel Prizes have been awarded for the cooling and trapping of atoms with lasers (Steven Chu, Claude Cohen-Tannoudji, William D. Phillips in 1997), and for the subsequent achievement of Bose–Einstein condensation in a dilute gas of trapped atoms (Eric A. Cornell, Wolfgang Ketterle, Carl E. Wieman in 2001). Although the topic of cooling and trapping was covered in the AIP Handbook, Bose–Einstein condensation was barely mentioned. Since then, the literature has exploded to nearly 2500 papers on Bose–Einstein condensation alone. Similarly, the topics of quantum information and quantum computing barely existed in 1995, and have since become rapidly growing segments of the physics literature. Entirely new topics such as "fast light" and "slow light" have emerged. Techniques for both high precision theory and measurement are opening the possibility to detect a cosmological variation of the fundamental constants with time. All of these topics hold the promise of important engineering and technological applications that come with advances in fundamental science. The more established areas of AMO Physics continue to provide the basic data and broad understanding of a great wealth of underlying processes needed for studies of the environment, and for astrophysics and plasma physics.


Prof. Gordon W. F. Drake

These changes and advances provide more than sufficient justification to prepare a thoroughly revised and updated *Atomic, Molecular and Optical Physics Handbook* for the Springer Handbook Program. The aim is to present the basic ideas, methods, techniques and results of the field at a level that is accessible to graduate students and other researchers new to the field. References are meant to be a guide to the literature, rather than a comprehensive bibliography. Entirely new chapters have been added on Bose–Einstein condensation, quantum information, variations of the fundamental constants, and cavity ring-down spectroscopy. Other chapters have been substantially expanded to include new topics such as fast light and slow light. The intent is to provide a book that will continue to be a valuable resource and source of inspiration for both students and established researchers.

I would like to acknowledge the important role played by the members of the Advisory Board in their continuing support of this project, and I would especially like to acknowledge the talents of Mark Cassar as Assistant Editor. In addition to keeping track of the submissions and corresponding with authors, he read and edited the new material for every chapter to ensure uniformity in style and scientific content, and he composed new material to be added to some of the chapters, as noted in the text.

February 2005 Gordon W. F. Drake

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Springer Handbook of Atomic, Molecular, and Optical Physics
Organization of the Handbook

Part A gathers together the mathematical methods applicable to a wide class of problems in atomic, molecular, and optical physics. The application of angular momentum theory to quantum mechanics is presented. The basic tenet that isolated physical systems are invariant to rotations of the system is thereby implemented into physical theory. The powerful methods of group theory and second quantization show how simplifications arise if the atomic shell is treated as a basic structural unit. The well established symmetry groups of quantum mechanical Hamiltonians are extended to the larger compact and noncompact dynamical groups. Perturbation theory is introduced as a bridge between an exactly solvable problem and a corresponding real one, allowing approximate solutions of various systems of differential equations. The consistent manner in which the density matrix formalism deals with pure and mixed states is developed, showing how the preparation of an initial state as well as the details regarding the observation of the final state can be treated in a systematic way. The basic computational techniques necessary for accurate and efficient numerical calculations essential to all fields of physics are outlined and a summary of relevant software packages is given. The ever present one-electron solutions of the nonrelativistic Schrödinger equation and the relativistic Dirac equation for the Coulomb potential are then summarized.

Part A Mathematical Methods

Part B presents the main concepts in the theoretical and experimental knowledge of atomic systems, including atomic structure and radiation. Ionization energies for neutral atoms and transition probabilities of selected neutral atoms are tabulated. The computational methods needed for very high precision approximations for helium are summarized. The physical and geometrical significance of simple multipoles is examined. The basic nonrelativistic and relativistic theory of electrons and atoms in external magnetic fields is given. Various properties of Rydberg atoms in external fields and in collisions are investigated. The sources of hyperfine structure in atomic and molecular spectra are outlined, and the resulting energy splittings and isotope shifts given. Precision oscillator strength and lifetime measurements, which provide stringent experimental tests of fundamental atomic structure calculations, are discussed. Ion beam spectroscopy is introduced, and individual applications of ion beam techniques are detailed A basic description of neutral collisional line shapes is given, along with a discussion of radiation transfer in a confined atomic vapor. Many qualitative features of the Thomas–Fermi model are studied and its later outgrowth into general density functional theory delineated. The Hartree–Fock and multiconfiguration Hartree–Fock theories, along with configuration interaction methods, are discussed in detail, and their application to the calculation of various atomic properties presented. Relativistic methods for the calculation of atomic structure for general many-electron atoms are described. A consistent diagrammatic method for calculating the structure of atoms and the characteristics of different atomic

Part B Atoms

processes is given. An outline of the theory of atomic photoionization and the dynamics of the photon–atom collision process is presented. Those kinds of electron correlation that are most important in photoionization are emphasized. The process of autoionization is treated as a quasibound state imbedded in the scattering continuum, and a brief description of the main elements of the theory is given. Green's function techniques are applied to the calculation of higher order corrections to atomic energy levels, and also of transition amplitudes for radiative transitions of atoms. Basic quantum electrodynamic calculations, which are needed to explain small deviations from the solution to the Schrödinger equation in simple systems, are presented. Comparisons of precise measurements and theoretical predictions that provide tests of our knowledge of fundamental physics are made, focussing on several quantitative tests of quantum electrodynamics. Precise measurements of parity nonconserving effects in atoms could lead to possible modifications of the Standard Model, and thus uncover new physics. An approach to this fundamental problem is described. The problem of the possible variation of the fundamental constants with time is discussed in relation to atomic clocks and precision frequency measurements. The most advanced atomic clocks are described, and the current laboratory constraints on these variations are listed.

Part B Atoms

Part C begins with a discussion of molecular structure from a theoretical/computational perspective using the Born–Oppenheimer approximation as the point of departure. The key role that symmetry considerations play in organizing and simplifying our knowledge of molecular dynamics and spectra is described. The theory of radiative transition probabilities, which determine the intensities of spectral lines, for the rotationally-resolved spectra of certain model molecular systems is summarized. The ways in which molecular photodissociation is studied in the gas phase are outlined. The results presented are particularly relevant to the investigation of combustion and atmospheric reactions. Modern experimental techniques allow the detailed motions of the atomic constituents of a molecule to be resolved as a function of time. A brief description of the basic ideas behind these techniques is given, with an emphasis on gas phase molecules in collision-free conditions. The semiclassical and quantal approaches to nonreactive scattering are outlined. Various quantitative approaches toward a description of the rates of gas phase chemical reactions are presented and then evaluated for their reliability and range of application. Ionic reactions in the gas phase are also considered. Clusters, which are important in many atmospheric and industrial processes, are arranged into six general categories, and then the physics and chemistry common to each category is described. The most important spectroscopic techniques used to study the properties of molecules are presented in detail.

Part C Molecules

Part D collects together the topics and approaches used in scattering theory. A handy compendium of equations, formulae, and expressions for the classical, quantal, and semiclassical approaches to elastic scattering is given; reactive systems and model potentials are also considered. The dependence of scattering processes on the angular orientation of the reactants and products is discussed through the analysis of scattering experiments which probe atomic collision theories at a fundamental level.

Part D Scattering Theory

The detailed quantum mechanical techniques available to perform accurate calculations of scattering cross sections from first principles are presented. The theory of elastic, inelastic, and ionizing collisions of electrons with atoms and atomic ions is covered and then extended to include collisions with molecules. The standard scattering theory for electrons is extended to include positron collisions with atomic and molecular systems. Slow collisions of atoms or molecules within the adiabatic approximation are discussed; important deviations from this model are presented in some detail for the low energy case. The main methods in the theoretical treatment of ion-atom and atom–atom collisions are summarized with a focus on intermediate and high collision velocities. The molecular structure and collision dynamics involved in ion–atom charge exchange reactions is studied. Both the perturbative and variational capture theories of the continuum distorted wave model are presented. The Wannier theory for threshold ionization is then developed. Studies of the energy and angular distribution of electrons ejected by the impact of high-velocity atomic or ionic projectiles on atomic targets are overviewed. A useful collection of formulae, expressions, and specific equations that cover the various approaches to electron-ion and ion-ion recombination processes is given. A basic theoretical formulation of dielectronic recombination is described, and its importance in the interpretation of plasma spectral emission is presented. Many of the equations used to study theoretically the collisional properties of both charged and neutral particles with atoms and molecules in Rydberg states are collected together; the primary approximations considered are the impulse approximation, the binary encounter approximation, and the Born approximation. The Thomas mass-transfer process is considered from both a classical and a quantal perspective. Additional features of this process are also discussed. The theoretical background, region of validity, and applications of the classical trajectory Monte Carlo method are then delineated. One-photon processes are discussed and aspects of line broadening directly related to collisions between an emitting, or absorbing, atom and an electron, a neutral atom or an atomic ion are considered.

Part D Scattering Theory

Part E focuses on the experimental aspects of scattering processes. Recent developments in the field of photodetachment are reviewed, with an emphasis on accelerator-based investigations of the photodetachment of atomic negative ions. The theoretical concepts and experimental methods for the scattering of low-energy photons, proceeding primarily through the photoelectric effect, are given. The main photon–atom interaction processes in the intermediate energy range are outlined. The atomic response to inelastic photon scattering is discussed; essential aspects of radiative and radiationless transitions are described in the two-step approximation. Advances such as cold-target recoil-ion momentum spectroscopy are also touched upon. Electron–atom and electron–molecule collision processes, which play a prominent role in a variety of systems, are presented. The discussion is limited to electron collisions with gaseous targets, where single collision conditions prevail, and to low-energy impact processes. The physical principles and experimental methods used to investigate low energy ion–atom collisions are outlined. Inelastic processes which occur in collisions between fast, often highly charged, ions and atoms, are described. A summary of the methods commonly employed in scattering experiments

Part E Scattering Experiment

involving neutral molecules at chemical energies is presented. Applications of single-collision scattering methods to the study of reactive collision dynamics of ionic species with neutral partners are discussed.

Part F presents a coherent collection of the main topics and issues found in quantum optics. Optical physics, which is concerned with the dynamical interactions of atoms and molecules with electromagnetic fields, is first discussed within the context of semiclassical theories, and then extended to a fully quantized version. The theoretical techniques used to describe absorption and emission spectra using density matrix methods are developed. Applications of the dark state in laser physics is briefly mentioned. The basic concepts common to all lasers, such as gain, threshold, and electromagnetic modes of oscillation are described. Recent developments in laser physics, including single-atom lasers, two-photon lasers, and the generation of attosecond pulses are also introduced. The current status of the development of different types of lasers – including nanocavity, quantum-cascade and free-electron lasers – are summarized. The important operational characteristics, such as frequency range and output power, are given for each of the types of lasers described. Nonlinear processes arising from the modifications of the optical properties of a medium due to the passage of intense light beams are discussed. Additional processes that are enabled by the use of ultrashort or ultra-intense laser pulses are presented. The concept of coherent optical transients in atomic and molecular systems reviewed; homogeneous and inhomogeneous relaxation in the theory are properly distinguished. Multiphoton and strong-field processes are given a theoretical description. A discussion of the generation of sub-femtosecond pulses is also included. General and specific theories for the control of atomic motion by light are presented. Various traps used for the cooling and trapping of charged and neutral particles and their applications are discussed. The fundamental physics of dilute quantum degenerate gases is outlined, especially in connection with Bose–Einstein condensation. de Broglie optics, which concerns the propagation of matter waves, is presented with a concentration on the underlying principles and the illustration of these principles. The fundamentals of the quantized electromagnetic field and applications to the broad area of quantum optics are discussed. A detailed description of the changes in the atom–field interaction that take place when the radiation field is modified by the presence of a cavity is given. The basic concepts needed to understand current research, such as the EPR experiment, Bell's inequalities, squeezed states of light, the properties of electromagnetic waves in cavities, and other topics depending on the nonlocality of light are reviewed. Applications to cryptography, tunneling times, and gravity wave detectors are included, along with recent work on "fast light" and "slow light." Correlations and quantum superpositions which can be exploited in quantum information processing and secure communication are delineated. Their link to quantum computing and quantum cryptography is given explicitly.

Part F Quantum Optics

Part G is concerned with the various applications of atomic, molecular, and optical physics. A summary of the processes that take place in photoionized gases, collisionally ionized gases, the diffuse interstellar medium, molecular clouds, circumstellar shells, supernova ejecta, shocked regions, and the early

Part G Applications

Universe are presented. The principal atomic and molecular processes that lead to the observed cometary spectra, as well as the needs for basic atomic and molecular data in the interpretation of these spectra, are focused on. The basic methods used to understand planetary atmospheres are given. The structure of atmospheres and their interaction with solar radiation are detailed, with an emphasis on ionospheres. Atmospheric global change is then studied in terms of the applicable atomic and molecular processes responsible for these changes. A summary of the well-known prescriptions for atomic structure and ionization balance, and a discussion of the modified transition rates for ions in dense plasmas are given. A review of current simulations being used to address a wide array of issues needed to accurately describe atoms in dense plasmas is also presented. The main concepts and processes of the physics and chemistry of the conduction of electricity in ionized gases are described. The physical models and laser diagnostics used to understand combustion systems are presented. Various applications of atomic and molecular physics to phenomena that occur at surfaces are reviewed; particular attention is placed on the application of electron- and photon-atom scattering processes to obtain surface specific structural and spectroscopic information. The effect of finite nuclear size on the electronic energy levels of atoms is also detailed; and conversely, the electronic structure effects in nuclear physics are discussed. A discussion of the concepts needed in the operation of charged particle detectors and in describing radiation effects is introduced. The description is restricted to fast charged particles. The key topics in basic radiation physics are then treated, and illustrative examples are given.

Part G Applications

Contents

Part A Mathematical Methods

4 Dynamical Groups

5 Perturbation Theory

6 Second Quantization

7 Density Matrices

8 Computational Techniques

9 Hydrogenic Wave Functions

Part B Atoms

10 Atomic Spectroscopy

11 High Precision Calculations for Helium

12 Atomic Multipoles

13 Atoms in Strong Fields

14 Rydberg Atoms

15 Rydberg Atoms in Strong Static Fields

16 Hyperfine Structure

17 Precision Oscillator Strength and Lifetime Measurements

24 Photoionization of Atoms

25 Autoionization

26 Green's Functions of Field Theory

27 Quantum Electrodynamics

Part C Molecules