

Handbook of Atomic, Molecular, and Optical Physics: Chapter Summaries

This document provides a brief summary of the contents of each of the chapters in the Handbook of Atomic, Molecular and Optical Physics. The divisions into the major subject areas of Mathematical Methods, Atoms, Molecules, Scattering Theory, Scattering Experiment, Quantum Optics, and Applications are indicated. The overall philosophy and goals of the book are described separately in the Preface.

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1 Units and Constants

William E. Baylis, Gordon W. F. Drake

The first chapter provides a handy reference for the currently accepted values for the funda-

mental constants in SI units, and their connections with the system of atomic units widely used in the calculation of atomic and molecular properties.

A Mathematical Methods

The next group of chapters gathers together the mathematical methods applicable to a wide class of problems in atomic, molecular, and optical physics.

2 Angular Momentum Theory

James D. Louck

The first chapter of this section presents the application of the powerful methods of angular momentum algebra to quantum mechanics. The intent is to provide a convenient reference for the most important techniques as they are applied to the calculation of matrix elements, and the analysis of angular momentum couplings. The basic tenet that isolated physical systems are invariant with respect to rotations of the system is thereby implemented into physical theory.

3 Group Theory for Atomic Shells

Brian R. Judd

The broadly useful methods of group theory and second quantization are introduced in this chapter, beginning with the basic definitions of Lie groups and their irreducible representations, unitary group methods in the theory of complex spectra, and Young Tableaux representations. Particularly important are the simplifications that arise from the use of the generalized Wigner–Eckart theorem and Casimir’s operator in the calculation of matrix elements involving partly filled shells of equivalent electrons. The chapter also discussed the accidental degeneracy of the hydrogen atom in terms of the $SO(4)$ symmetry of the Hamiltonian.

4 Dynamical Groups

Josef Paldus

The conventional symmetry groups of quantum mechanical Hamiltonians are extended in this chapter to the larger compact and noncompact dynamical groups. Simple examples are provided by the Lie algebras associated with $SO(4)$ and its extensions. An important aim and motivation for these group theoretical methods is to obtain purely algebraic solutions to quantum mechanical problems such as the N -dimensional hydrogen atom, Klein–Gordon equation and Dirac equation, including perturbations due to external electric and magnetic fields. Many other similar problems are discussed, and the Clifford algebra unitary group approach is discussed in detail. The material provides an excellent introduction to the main ideas, and a guide to the literature.

5 Perturbation Theory

Josef Paldus

Perturbation theory is introduced as a bridge between the relatively few problems that can be solved exactly, and the many others that are of physical interest. The treatment begins with basic definitions and elementary concepts, and then proceeds to discuss the Brillouin–Wigner and Rayleigh–Schrödinger perturbation theory for degenerate and nondegenerate systems. The chapter then introduces the reader to the powerful techniques of many-body perturbation theory for atomic structure calculations in second-quantized form. The results (including Møller–Plesset and Epstein–Nesbet perturbation theory) are cast in diagrammatic form, and Wick’s Theorem is introduced. The chapter includes a discussion of time-dependent perturbation theory and the perturbation expansion of the evolution operator in the interaction representation. The treatment provides a particularly valuable introduction to the literature, including the basic formalism of scattering theory.

6 Second Quantization

Brian R. Judd

This chapter provides an extended discussion of the formalism of second quantization and its applications to

problems in atomic structure and scattering theory. The particular focus is on the coupling of creation and annihilation operators to form tensors of various ranks, and the related coefficients of fractional parentage, and quasi-spin operators for fermions and bosons.

7 Density Matrices

Klaus Bartschat

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. Applications are described involving coherence and correlation phenomena, alignment and orientation and their effect on the polarization of emitted radiation, quantum beat spectroscopy, optical pumping, and scattering processes, particularly when spin-polarized projectiles and/or targets take part.

8 Computational Techniques

David R. Schultz, Michael R. Strayer

The basic computational techniques necessary for the accurate and efficient numerical calculations essential to all fields of physics are outlined and a summary of relevant software packages is given.

9 Hydrogenic Wave Functions

Robert N. Hill

This chapter provides a convenient reference for the solutions and properties of the one-electron nonrelativistic Schrödinger equation, and the one-electron relativistic Dirac equation, for the Coulomb potential. The results are related to standard reference works such as Abramowitz and Stegun, the Bateman project, Gradshteyn and Ryzhik, Jahnke and Emde, Luke, Magnus, Oberhettinger and Soni, Olver, and Szego. The section on special functions contains many of the formulas which are needed to check the results quoted in the other sections, together with a number of other useful formulas. It includes a brief introduction to asymptotic methods. A reference to the numerical evaluation of special functions is given.

B Atoms

10 Atomic Spectroscopy

William C. Martin, Wolfgang L. Wiese

This chapter outlines the main concepts of atomic structure, with some emphasis on terminology and notation. Atomic radiation is discussed; in particular the wavelengths, intensities, and shapes of spectral lines, including continuous spectra. Updated tabulations of ionization energies for the neutral atoms and transition probabilities for persistent lines of selected neutral atoms are given. References to additional atomic spectroscopic data are included.

11 High Precision Calculations for Helium

Gordon W. F. Drake

Exact analytic solutions to the Schrödinger equation are known only for atomic hydrogen, and other equivalent two-body systems (see Chap. 9). However, very high precision approximations are now available for helium, that are essentially exact for all practical purposes. This chapter summarizes the computational methods and tabulates numerical results for the ground state and several singly excited states. The chapter includes a discussion of relativistic and quantum electrodynamic corrections, as well as asymptotic expansion methods for Rydberg states. Similar methods can be applied to other three-body problems.

12 Atomic Multipoles

William E. Baylis

This chapter applies the density matrix formalism to a typical atomic experiment involving the preparation of an atomic or molecular ensemble, its perturbation by a combination of collisions and external fields, and the characterization of the perturbed system through detection of emitted or scattered particles or quanta. The time development of the system may depend on interactions among the atoms of the ensemble with each other, with external fields, and with external perturbers. Significant simplifications can usually be made to reduce the complexity.

13 Atoms in Strong Fields

S. P. Goldman, Mark M. Cassar

A new regime of phenomena appears when the interaction of atomic electrons with external electric or

magnetic fields becomes large in comparison with the Coulomb interaction with the nucleus. This chapter discusses the Landau levels that appear in a strong magnetic field for both the nonrelativistic (Schrödinger) and relativistic (Dirac) cases, as well as the normal Stark and Zeeman effects for weak and moderately strong fields.

14 Rydberg Atoms

Thomas F. Gallagher

Rydberg atoms are those in which the valence electron is in a state of high principal quantum number n .

Since the 1970s they have been studied mostly for two reasons. First, Rydberg states are at the border between bound states and the continuum, and any process which can result in either excited bound states or ions and free electrons usually leads to the production of Rydberg states. Second, the exaggerated properties of Rydberg atoms allow experiments to be done which would be difficult or impossible with normal atoms. This chapter discusses the specialized techniques that have been developed to deal with Rydberg atoms, such as the quantum defect theory, optical excitation and radiative lifetimes, cavity effects, the Stark and Zeeman effects for Rydberg atoms, and field ionization. The chapter particularly focuses on topics of current research interest.

15 Rydberg Atoms in Strong Static Field

Thomas F. Gallagher

Confronting classical and quantum mechanics in systems in which the classical motion is chaotic is one of the fundamental problems of this decade, as evidenced by the enormous outpouring of research on this subject. In particular, the attention of many atomic physicists and nonlinear dynamicists has been focused on electron dynamics and spectroscopy in highly excited Rydberg atoms in strong external fields. This chapter discusses the more specialized research topics at the interface between classical and quantum physics.

16 Hyperfine Structure

Guy T. Emery

Hyperfine structure in atomic and molecular spectra is a result of the interaction between electronic degrees of freedom and nuclear properties other than the dominant nuclear Coulomb field. It includes splittings of

energy levels (and thus of spectral lines) from magnetic dipole and electric quadrupole interactions (and higher multipoles, on occasion). This chapter covers hyperfine structure and the related isotope shifts, including the so called field effect in the isotope shift due to finite nuclear size. Studies of hyperfine structure can be used to probe nuclear properties, but they are an equally important probe of the structure of atomic systems, providing especially good tests of atomic wave functions near the nucleus. There are also isotope shifts owing to the mass differences between different nuclear species, and the study of these shifts provides useful atomic information, especially about correlations between electrons. Recent theoretical progress in the calculation of hyperfine structure from first principles is discussed.

17 Precision Oscillator Strength and Lifetime Measurements

Lorenzo J. Curtis

A traditional area of atomic spectroscopy has been the measurement of oscillator strengths and atomic lifetimes. These quantities determine the strength (brightness) of spectral lines, and hence they contain important information about the excitation conditions responsible for the light being emitted. This chapter discussed the principal experimental techniques available for measurements of this type and the most important results.

18 Ion Beam Spectroscopy

Eric H. Pinnington, Elmar Träbert

This chapter discussed the particular advantages that a beam of ionized atoms has as a spectroscopic source. Unlike arcs, sparks and high temperature plasmas, the ions in a beam can be studied in an environment that is free of electric and magnetic fields, and relatively free of interparticle collisions. Standard accelerator techniques from nuclear physics may be used to produce a well-collimated, mass-analyzed beam of ions having a low velocity spread. In principle, virtually any charge state of any element, isotopically pure if required, can be obtained, given the appropriate equipment. Finally, the well-defined velocity of the beam permits the study of processes evolving in time in terms of their spatial evolution along the beam. This is particularly important in the case of lifetime measurements, discussed in the previous chapter. An experiment can involve an ion energy as low as a few keV or as high as several GeV. However, in this article the individual applications of ion beam

techniques in atomic physics will be classified by the means used (foil, gas, laser etc.) to excite the ions, since this better defines the type of research in each case.

19 Line Shapes and Radiation Transfer

Alan Gallagher

This chapter focuses on the shapes of collisionally broadened atomic lines, and the wealth of information that can be obtained from them. The chapter begins with elementary principles of line-shape theory, including the impact and static pictures and how they can be reconciled through Fourier integral theory, and more modern theories based on a quantum description. Many of the commonly used approximation methods are discussed and reviewed, such as the quasi-static approximation, and the stationary phase approximation. Also included are radiation-trapping effects, and Holstein–Biberman theory.

20 Thomas–Fermi and other Density–Functional Theories

John D. Morgan III

Thomas–Fermi theory provides a simplified description of an atom or atomic ion with a large nuclear charge Z and a large number of electrons N . Many qualitative features of this model can be studied analytically, and the precise solution can be found by solving numerically a nonlinear ordinary differential equation. Lenz demonstrated that this equation for the electrostatic potential could be derived from a variational expression for the energy as a functional of the density. The chapter discusses Refinements to Thomas–Fermi theory to include a term in the energy functional to account for electron exchange effects introduced by Dirac, and nonlocal gradient corrections to the kinetic energy introduced by von Weizsäcker. The basic ideas of the very widely used density functional theory are discussed.

21 Atomic Structure: Multiconfiguration Hartree–Fock Theories

Charlotte F. Fischer

The Hartree–Fock (H.F) approximation provides the best possible solution to the many particle Schrödinger equation within the independent particle central-field approximation. This chapter provides a basic introduction to the H.F. approximation, followed by systematic methods to improve it through the mixing of different atomic configurations (configuration interaction). The chapter

also discusses the lowest order relativistic corrections to the Schrödinger equation in terms of the Breit interaction. The material provides an excellent introduction to the vast literature in this area.

22 Relativistic Atoms Structure

Ian P. Grant

Relativistic quantum mechanics is required for the description of atoms and molecules whenever their orbital electrons probe regions of space with high potential energy near the atomic nuclei. Primary effects of a relativistic description include changes to spatial and momentum distributions; spin-orbit interactions; quantum electrodynamic corrections such as the Lamb shift; and vacuum polarization. The emphasis in this chapter is on relativistic methods for the calculation of atomic structure for general many-electron atoms based on an effective Hamiltonian derived from QED. The chapter provides an understanding of the Dirac equation, its solutions and their numerical approximation for the study of many-electron systems.

23 Many-Body Theory of Atomic Structure and Processes

M. Ya. Amusia

All atoms except hydrogen are many-body systems in which the interelectron interaction plays an important or even decisive role. The aim of this chapter is to describe a consistent method for calculating the structure of atoms and the characteristics of different atomic processes, by applying perturbation theory to take into account the interelectron interaction. This method involves drawing a characteristic diagram based on the structure or process. This is then used to create an analytical expression to the lowest order in the interelectron interaction. Higher-order corrections are subsequently generated.

24 Photoionization of Atoms

Anthony F. Starace.

In the process of photoionization, an atom is ionized by the absorption of a photon with sufficient energy to eject an electron. This chapter outlines the theory of atomic photoionization, and the dynamics of the photon–atom collision process. Those kinds of electron correlation that are most important in photoionization are emphasized, although many qualitative features can be understood within a central field model. The

particle–hole type of electron correlations are discussed, as they are by far the most important for describing the single photoionization of atoms near ionization thresholds.

25 Autoionization

Aaron Temkin, Anand K. Bhatia

The phenomenon of autoionization corresponds to a scattering resonance that can be thought of as a quasi-bound state imbedded in the scattering continuum. The state can subsequently decay with the emission of an electron, leaving behind an atomic ion. The inverse process of dielectronic recombination greatly accelerates the rate of recombination in plasmas. The process is rigorously a part of the scattering continuum, but, due mostly to the work of Feshbach, a rigorous formulation can be established whereby the main element of the theory can be made into a bound state problem with the scattering elements built around it. The major constituent of both these features is accomplished with projection operators. A brief description of the above elements of the theory, centered around projection operators, is the aim of this chapter.

26 Green's Functions of Field Theory

Gordon Feldman, Thomas Fulton

This chapter describes the mathematical apparatus of Green's function techniques as applied to problems in atomic physics; specifically to the calculation of higher order correlation, Breit, and radiative corrections to energy levels, and also of transition amplitudes for radiative transitions of atoms. The methods are gauge invariant at every level of approximation.

27 Quantum Electrodynamics

Jonathan R. Sapirstein

Quantum Electrodynamics (QED) is the underlying theory of atomic and molecular physics. In the nonrelativistic limit, QED reduces to the Schrödinger equation, and the extra physics in QED in general is quite small, being suppressed by powers of the fine structure constant α . The theory is needed to explain small deviations from the solutions to the Schrödinger equation. This chapter provides a general overview, and in particular discusses a single electron in a constant magnetic field, one-electron atoms, and helium. Larger deviations occur for highly charged ions, and also for high-energy scattering of electrons and photons.

28 Tests of Fundamental Physics

Peter J. Mohr, Barry N. Taylor

This Chapter describes comparisons of precise measurements and theoretical predictions that provide tests of our knowledge of fundamental physics. The focus is on several quantitative tests of quantum electrodynamics (QED). The basic formulation of the theory of QED and calculational methods are discussed in the previous chapter. Here, only the end results of calculations are collected, numerically evaluated, and compared with the corresponding experiments.

29 Parity Nonconserving Effects in Atoms

Jonathan R. Sapirstein

It was shown in 1957 that weak interaction processes are not invariant under parity inversion. In 1974 the Bouchiat, in a paper that laid the foundation for the field, showed that the exceedingly small effects of parity non-conservation (PNC) were enhanced in heavy atoms with atomic number Z by a factor of Z^3 . While still very small, this effect has been observed in a variety of heavy

atoms, specifically cesium ($Z = 55$), thallium ($Z = 81$), lead ($Z = 82$), and bismuth ($Z = 83$). The accurate calculation of the electronic structure of such atoms is, of course, a very challenging atomic physics problem, and such calculations must be carried out before the experiments can be interpreted in terms of particle physics. This chapter discusses the fundamental ideas involved and recent progress.

30 Variation of the Fundamental Constants

Savely G. Karshenboim, Victor Flambaum, Ekkehard Peik

There has been much recent speculation, and some astrophysical evidence, that the so-called 'fundamental' constants may in fact be varying on a cosmological time scale. This chapter presents a general theoretical framework for the discussion of the variation of the fundamental constants with time. Recent work 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 summarized.

C Molecules

31 Molecular Structure

David R. Yarkony

The discussion of molecules begins with an understanding of molecular structure. This Chapter considers issues in molecular structure from a theoretical/computational perspective using the Born–Oppenheimer approximation as the point of departure.

excitation that lead to the emission of light. This Chapter summarizes the theory of radiative transition probabilities or intensities for rotationally-resolved spectra for diatomic, linear, symmetric-top, and asymmetric-top molecules. Generality and symmetry relations are emphasized.

32 Molecular Symmetry and Dynamics

William G. Harter

Symmetry considerations play a key role in organizing and simplifying our knowledge of molecules. This discussion of molecular dynamics and spectra mainly involves molecular rotation and properties of rotationally excited molecules with applications to excited vibrational, and in some cases electronic, states.

34 Molecular Photodissociation

Abigail J. Dobbyn, David H. Mordant, Reinhard Schinke

In the process of photodissociation, a molecule is induced to break up into fragments by the absorption of a photon of light. The ways in which the photoinitiated fragmentation of a bound molecule, or molecular photodissociation, is studied in the gas phase are outlined. The results presented are particularly relevant to the investigation of combustion and atmospheric reactions.

33 Radiative Transition Probabilities

David L. Huestis

Radiative transition probabilities determine the intensities of Spectral lines, and hence the conditions of

35 Time-Resolved Molecular Dynamics

Volker Engel

Modern experimental techniques allow the detailed motions of the Atomic constituents of a molecule to be

resolved as a function of time. Although time-resolved experiments have been performed on a diverse number of molecular systems, the principles of the experiments are more or less the same. A brief description of the basic ideas is given, with an emphasis on gas phase molecules in collision-free conditions.

36 Nonreactive Scattering

David R. Flower

The rates of all chemical processes are determined by the cross sections for various basic scattering processes. As a first step, the semiclassical and quantal approaches to nonreactive scattering are outlined. This includes the specific symmetries, related conservation laws, and particular coordinate systems, as well as prescriptions for determining the various matrix elements needed for a given calculation.

37 Gas Phase Reactions

Eric Herbst

The next step beyond nonreactive scattering is the study of gas phase reactions. Various quantitative approaches toward a description of the rates of gas phase chemical processes are presented and then evaluated for their reliability and range of application.

38 Gas Phase Ionic Reactions

Nigel G. Adams

Ionic reactions in the gas phase are considered from a straightforward three-part perspective: the initial interaction, in which the colliding particles are drawn together; the reaction intermediate and transition state, in which reactants are transformed into products; and the weakening interaction as the product particles separate.

39 Clusters

Mary L. Mandich

Many atmospheric and industrial processes involve clusters containing tens to hundreds of molecules. This chapter arranges clusters into six general categories, and then proceeds to describe the physics and chemistry common to each category, placing particular emphasis on the unique properties of clusters owing to their finite size and finite lattice structure.

40 Infrared Spectroscopy

Henry Buijs

This is the first of five chapters describing the most important spectroscopic techniques used to study the properties of molecules. The use of infrared spectroscopy, which consists of the measurement of interactions of waves of the infrared radiation with matter, to elucidate molecular structure and to identify and quantify different molecular species in a sample, are detailed.

41 Lasers Spectroscopy in the Submillimeter and Far-Infrared Regions

Kenneth M. Evenson†, John M. Brown

Experimental techniques for the production and detection of tunable and fixed frequency submillimeter and infrared radiation are described; applications to astrophysical and upper-atmospheric studies are then detailed.

42 Spectroscopic Techniques: Lasers

Paul Engelking

The basic operating principles, configurations, and characteristic parameters of lasers are given. Laser designs are discussed and then the details of the interaction of the laser light with matter delineated.

43 Spectroscopic Techniques: Cavity-Enhanced Methods

Barbara A. Paldus, Alexander A. Kachanov

The aim of this chapter is to present the fundamentals of cavity-enhanced spectroscopy and the various modifications and extensions that have been developed for its application in a wide range of experimental settings; particular emphasis is placed on cavity ring-down spectroscopy as a method of achieving enhanced sensitivity and precision.

44 Spectroscopic Techniques: Ultraviolet

Glenn Stark, Peter L. Smith

In this chapter, we review the instrumentation available for uv spectroscopy, concentrating on the vuv, where special instrumentation is necessary. Recent advances are stressed, particularly in the areas of synchrotron radiation and the production of vuv laser light.

D Scattering Experiment

45 Elastic Scattering: Classical, Quantal, and Semiclassical

M. Raymond Flannery

Scattering cross sections determine the rates at which gas phase processes and chemical reactions happen, whether in the atmosphere, or in an industrial reactor. This chapter provides a handy compendium of equations, formulae, and expressions for the classical, quantal, and semiclassical approaches to elastic scattering. Reactive systems and model potentials are also considered.

46 Orientation and Alignment in Atomic and Molecular Collisions

Nils Andersen

The dependence of scattering processes on the angular orientation of the reactants and products provides a sensitive test of the underlying scattering mechanisms. This chapter discusses the analysis of scattering experiments which exploit the planar scattering symmetry in order to probe atomic collision theories at a more fundamental level.

47 Electron–Atom, Electron–Ion, and Electron–Molecule Collisions

Philip G. Burke

This chapter provides extensive coverage of the detailed quantum mechanical techniques available to perform accurate calculations of scattering cross sections from first principles. 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. Collisions of electrons and atoms in intense laser fields is also discussed.

48 Positron Collisions

Robert P. McEachran, Al D. Stauffer

The standard scattering theory for electrons is extended to include positron collisions with atomic and molecular systems. The basic theoretical methods, particular applications, and recent developments of cold trap-based positron beams are given.

49 Adiabatic and Diabatic Collision Processes at low Energies

Evgueni E. Nikitin

Slow collisions of atoms or molecules are of great interest in the study of Bose–Einstein condensates. Here, the added condition is that the de Broglie length of the relative velocity is much smaller than the effective range of the interaction potential. The adiabatic approximation is discussed; deviations from this model, which manifest themselves as transitions between adiabatic potential energy surfaces, are presented in some detail for the low energy case.

50 Ion–Atom and Atom–Atom Collisions

A. Lewis Ford, John F. Reading

The main concepts, terminology, and methods in the theoretical treatment of ion–atom and atom–atom collisions are summarized with a focus on intermediate and high collision velocities.

51 Ion–Atom Charge Reactions at low Energies

Muriel Gargaud, Ronald McCarroll

A discussion of the molecular structure and collision dynamics involved in ion–atom charge exchange reactions is presented. Two particular types of electron capture are discussed: one in which no change occurs in the core electron configuration and one in which there is a rearrangement of the core electron configuration.

52 Continuum Distorted Wave and Wannier Methods

Derrick S. F. Crothers, F. B. M. Copeland, J. T. Glass, Jim F. McCann, S. F. C. O'Rourke, Ruth T. Pedlow

The continuum distorted wave and Wannier methods provide important frameworks for the description of processes involving ionization. Both the perturbative and variational capture theories of the continuum distorted wave model are presented, including recent developments in third-order, relativistic, and magnetically quantized continuum distorted waves. A novel

ionization theory for low energies is also reported. The Wannier theory for threshold ionization is then developed, highlighting the below-threshold semiclassical theory for the study of doubly excited states and a more accurate variant of the semi-classical quantum-mechanical treatment.

53 Ionization in High Energy Ion–Atom Collisions

Joseph H. Macek, Steven T. Manson

When high-velocity atomic species interact with matter, they effect chemical and biological changes which originate with primary collision processes, usually the ejection of electrons. This chapter gives an overview of this primary process that has emerged from studies of the energy and angular distribution of electrons ejected by the impact of atomic or ionic projectiles on atomic targets. It seeks to highlight those features which are most ubiquitous.

54 Electron–Ion and Ion–Ion Recombination

M. Raymond Flannery

Electron–ion and ion–ion recombination processes are of key importance in understanding the properties of plasmas, whether they are in the upper atmosphere, the solar corona, or industrial reactors on earth. This is a collection of formulae, expressions, and specific equations that cover the various aspects, approximations, and approaches to electron–ion and ion–ion recombination processes.

55 Dielectric Recombination

Michael S. Pindzola, Donald C. Griffin, Nigel R. Badnell

The dielectronic recombination mechanism provides one of the most efficient recombination mechanisms in plasmas. A basic theoretical formulation of dielectronic recombination is given, along with comparisons with experiments with high- and low- Z ions. A brief discussion of DR's importance in the interpretation of plasma spectral emission is presented.

56 Rydberg Collisions: Binary Encounter, Born, and Impulse Approximations

E. J. Mansky

This chapter collects together many of the equations used to study theoretically the collisional properties of both charged and neutral particles with atoms and molecules in Rydberg states. The primary theoretical scattering approximations considered are the impulse approximation, the binary encounter approximation, and the Born approximation.

57 Mass Transfer at High Energies: Thomas Peak

James H. McGuire, Jack C. Straton, Takeshi Ishihara

The two-step mass transfer process known, as the Thomas process, is considered from both a classical and a quantal perspective. Additional features of this process – off-energy-shell effects, dispersion relations, destructive interference of peak amplitudes – are also discussed.

58 Classical Trajectory and Monte Carlo Techniques

R. E. Olson

The theoretical background, region of validity, and applications of the classical trajectory Monte Carlo method are the main focus of this Chapter. The use of modern vector- and parallel processors for detailed studies of collision processes is touched upon.

59 Collisional Broadening of Spectral Lines

Gillian Peach

The shape of spectral lines contains important information about the conditions of temperature and pressure in the source producing the radiation, whether it is a plasma reactor on earth, or a remote astrophysical object. One-photon processes are discussed and aspects of line broadening (pressure, Stark, and collisional broadening) directly related to collisions between an emitting (or absorbing) atom and an electron, a neutral atom or an atomic ion are considered.

E Scattering Theory

60 Photodetachment

David J. Pegg

The next several chapters focus on the experimental aspects of scattering processes, beginning with photodetachment. In the gaseous phase the photoelectric effect is referred to as either photoionization (atoms and positive ions) or photodetachment (negative ions). This chapter reviews recent developments in the field of photodetachment. The focus will be on accelerator-based investigations of the photodetachment of atomic negative ions.

61 Photon–Atom Interactions: Low Energy

Denise Caldwell, Manfred O. Krause

The theoretical concepts and experimental methods for the scattering of low-energy photons, proceeding primarily through the photoelectric effect, are given. Relativistic and higher-order effects are briefly discussed.

62 Photon–Atom Interactions: Intermediate Energy

Bernd Crasemann

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. Multi-electron photoexcitation that transcends the independent-electron model is briefly considered. Recent advances such as Cold-Target Recoil-Ion Momentum Spectroscopy (COLTRIMS) are also touched upon.

63 Electron–Atom and Electron–Molecule Collisions

Sandor Trajmar, William J. McConkey, Isik Kanik

Electron–atom and electron–molecule collision processes, which play a prominent role in a variety

of systems ranging from discharge or electron-beam lasers and plasma processing devices to aurorae and solar plasmas, are presented. The discussion is limited to electron collisions with gaseous targets, where single collision conditions prevail, and to low-energy impact processes.

64 Ion–Atom Scattering Experiments: Low Energy

Ronald Phaneuf

There has been tremendous progress in recent years in the laboratory study of ion–atom scattering processes. This chapter outlines the physical principles and experimental methods used to investigate low energy ion–atom collisions.

65 Ion–Atom Collisions – High Energy

Lew Cocke, Michael Schulz

This chapter deals with inelastic processes which occur in collisions between fast, often highly charged, ions and atoms, outlining some of the developments in this area over a very active past few decades.

66 Reactive Scattering

Arthur G. Suits, Yuan T. Lee

This chapter presents a résumé of the methods commonly employed in scattering experiments involving neutral molecules at chemical energies. These experiments include the study of intermolecular potentials, the transfer of energy in molecular collisions, and elementary chemical reaction dynamics.

67 Ion–Molecule Reactions

James M. Farrar

This chapter discusses applications of single-collision scattering methods to the study of reactive collision dynamics of ionic species with neutral partners.

F Quantum Optics

68 Light–Matter Interaction

Pierre Meystre

Optical physics is concerned with the dynamical interactions of atoms and molecules with electromagnetic fields. Semiclassical theories, which study the interaction of atoms with classical fields, are often said to comprise optical physics. A significant part of optical physics is the study of near-resonant atom–field interactions, and concentrates on nonperturbative dynamics, where the effects of the optical fields have to be kept to all orders. The atomic properties themselves are assumed to be known. The vast majority of problems in light–matter interactions can be treated quite accurately within semiclassical theories. The present chapter deals with more “traditional” aspects of optical physics.

69 Absorption and Gain Spectra

Stig Stenholm

This chapter develops theoretical techniques to describe absorption and emission spectra using semiclassical concepts and density matrix methods. The simplest cases are treated, with more realistic applications left to other chapters. Only steady-state spectroscopy is covered. Applications of the dark state in laser physics is briefly mentioned.

70 Laser Principles

Peter W. Milonni

Despite their great variety and range of power, wavelength, and temporal characteristics, all lasers involve certain basic concepts, such as gain, threshold, and electromagnetic modes of oscillation. In addition to these universal characteristics are features, such as Gaussian beam modes, that are important to such a wide class of devices that they must be included in any reasonable compendium of important laser concepts and formulas. We have therefore included here both generally applicable results as well as some more specific but widely applicable ones. Recent developments in the basic physics of lasers include the application of cavity QED techniques to produce a single-atom laser and a two-photon laser. Recent progress in the development of ultrashort pulses includes the generation of attosecond pulses by high-order harmonic generation.

71 Types of Lasers

Richard C. Powell

The laser is the basic tool for atomic and molecular spectroscopy and for elucidating fundamental properties of optics and optical interactions with matter. This chapter summarizes the current status of the development of different types of lasers including nanocavity, quantum-cascade and free-electron lasers emphasizing those that are commercially available. The important operational characteristics, such as frequency range and output power, are given for each of the types of lasers described herein.

72 Nonlinear Optics

Alexander L. Gaeta, Robert W. Boyd

Nonlinear optics is concerned with the propagation of intense beams of light through a material system. The optical properties of the medium can be modified by the intense light beam, leading to new processes that would not occur in a material that responded linearly to an applied optical field. These processes can lead to the modification of the spectral, spatial, or polarization properties of the light beam, or the creation of new frequency components, and are the focus of this chapter. Additional nonlinear optical processes are enabled by the use of ultra-short or ultra-intense laser pulses are discussed.

73 Coherent Transients

Joseph H. Eberly, Carlos R. Stroud Jr

Coherent optical transients are excited in atomic and molecular systems when a stable phase relation persists between an exciting light field and the system’s electronic response. The extreme sensitivity of phase-dependent effects is responsible for the many applications of optical transient techniques in atomic and molecular physics. Homogeneous and inhomogeneous relaxation in the theory of coherent transients are properly distinguished.

74 Multiphoton and Strong-Field Processes

Kenneth C. Kulander, M. Lewenstein

The excitation of atoms by intense laser pulses can be divided into two broad regimes: the first regime involves relatively weak optical laser fields of long duration, and the second involves strong fields of short duration. In the first case, the intensity is presumed to be high enough

for multiphoton transitions to occur. The resulting spectroscopy is not limited by the single-photon selection rules for radiative transitions. However, the intensity is still low enough for a theoretical description based on perturbations of field-free atomic states to be valid, and the time dependence of the field amplitude does not play an essential role. In the second case, the field intensities are too large to be treated by perturbation theory, and the time dependence of the pulse must be taken into account. A discussion on the generation of sub-femtosecond pulses is included.

75 Cooling and Trapping

Juha Javanainen

This chapter presents general and specific, for two- and multi-state atoms, theories for the control of atomic motion by light. Various traps used for the cooling and trapping of charged and neutral particles and their applications are discussed. The development based on the atom-field dressed states is followed only sparingly.

76 Quantum Degenerate Gases

Juha Javanainen

The achievement of Bose–Einstein condensation in dilute atomic gases has transformed the field of AMO physics. The purpose of this Chapter is to summarize the basic physics of dilute quantum degenerate gases. Emphasis is placed on AMO physics, in the vein of quantum optics. For the most part, the coverage is on elementary concepts and basic material.

77 De Broglie Optics

Carsten Henkel, Martin Wilkens

De Broglie optics concerns the propagation of matter waves, their reflection, refraction, diffraction and interference. This chapter concentrates on the principles of de Broglie optics. Illustrations of these principles will be presented mainly in the framework of atom optics. Regardless of the particle species, the theory of de Broglie optics divides into two distinct parts: the theory of dispersion and the theory of the optical phenomena.

78 Quantized Field Effects

Matthias Freyberger, Karl Vogel, Wolfgang P. Schleich, Robert F. O'Connell

This chapter discusses the fundamentals of the quantized electromagnetic field and applications to the broad

area of quantum optics. Mention is also made of how quantum optics has blossomed in several new directions particularly in the key role it is playing in recent investigations of the fundamentals of quantum theory and related applications. In particular, the superposition principle, entanglement, the quantum-classical interface and precision measurements have become very topical research areas, especially in respect to their relevance to quantum information processing.

79 Entangled Atoms and Fields: Cavity QED

Dieter Meschede, Axel Schenzle

This chapter is concerned with the changes in the atom–field interaction that take place when the radiation field is modified by the presence of a cavity. An atom in the vicinity of a plane perfect mirror serves as an example of cavity quantum electrodynamics. The primary focus in this chapter is the two extreme cases of weak coupling and strong coupling, as exemplified by spontaneous emission.

80 Quantum Optical Tests of the Foundations of Physics

Aephraim M. Steinberg, Paul G. Kwiat, Raymond Y. Chiao

The quantum nature of light gives rise to a wide variety of fascinating new phenomena that have many practical applications, as well as testing our understanding of fundamental physical principles. This chapter reviews 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. Applications to cryptography, tunneling times, and gravity wave detectors are included, along with recent work on “fast light” and “slow light.”

81 Quantum Information

Peter L. Knight, Stefan Scheel

Correlations and quantum superpositions can be exploited in quantum information processing and secure communication. This has led to an explosive growth of the subject, fueled by the long-term prospects of quantum computing and the nearer goal of quantum

G Applications

82 Applications of Atomic and Molecular Physics to Astrophysics

Adal Dalgarno, Stephen Lepp

Atomic and molecular physics provides the tools to analyze and understand the light we receive from remote objects in the universe. 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 Universe are presented.

83 Comets

Paul D. Feldman

Comets are small bodies of the solar system believed to be remnants of the primordial solar disk. Cometary volatiles are vaporized as their orbits bring them closer to the sun and it is solar radiation that initiates all of the processes that lead to the extended coma. All determinations of the volatile composition of the coma are derived from spectroscopic analysis. Detailed modeling is then used to infer the volatile composition of the cometary nucleus. This chapter focuses on the principal atomic and molecular processes that lead to the observed spectrum as well as the needs for basic atomic and molecular data in the interpretation of these spectra.

84 Aeronomy

J. L. Fox

The basic methods of AMO physics used to understand planetary atmospheres are given. The structure of atmospheres and their interaction with solar radiation are detailed, with an emphasis on ionospheres.

85 Applications of Atomic and Molecular Physics to Global Change

Kate P. Kirby, Kelly Chance

Knowledge of processes taking place in the atmosphere, oceans, land masses, and plant and animal populations, as well as the interactions between these various earth-system components is essential to an overall understanding of global change – both natural and human-induced. The processes of atomic and molecular physics find greatest application in the area of atmospheric global change. The two major issues which have received significant attention in both the media and the

scientific literature are: (1) global warming, due to the buildup of infrared-active gases; and (2) stratospheric ozone depletion due to an enhancement of destructive catalytic cycles. Although both of these problems are thought to be caused by atmospheric pollutants due to industrialized human society, the general problem of air pollution and its direct effects on plant and animal populations will not be addressed here.

86 Atoms in Dense Plasma

Jon C. Weisheit, Michael S. Murillo

This chapter focuses on partially ionized matter in which important atomic phenomena are influenced by a dense plasma environment. The densities in many laboratory and astrophysical plasmas are high enough to invalidate the presumption of isolated systems. These plasmas are the basis of world-wide inertial confinement fusion (ICF) efforts. The topics addressed here are needed for understanding situations with local thermal equilibrium as well as those without. After characterizing the perturbing plasma environment, we summarize well-known prescriptions for atomic structure and ionization balance, and then discuss modified transition rates for ions in dense plasmas. Finally, we review how simulations are now being used to address a wide array of issues needed to accurately describe atoms in dense plasmas. No single experimental methodology or theoretical construct suffices to explore all aspects of the plasma state.

The present topic is an important part of what is now being termed “high energy-density physics” (HEDP). Conventionally this interdisciplinary subject, which involves collective and/or non-linear phenomena in many-body systems, is defined as the study of matter in regimes where the total pressure exceeds one megabar.

87 Conduction of Electricity in Gases

Alan Garscadden

The conduction of electricity through gases was responsible for many of the fundamental discoveries in atomic and molecular physics; gas discharge lighting is essential to every night operations; gas discharge lasers are still important in research and manufacturing; and all of advanced microelectronics depends on plasma enhanced processing. The physics and chemistry of the conduction of electricity in ionized gases involves the interactions of the electrons and ions in the gas among themselves, with ground-state and excited-state gas atoms or molecules,

with any surfaces that may be present, and with any electric or magnetic fields that are externally applied or generated by movement of the charged species. Topics covered: the electron-velocity distribution and its effect on various measurements involving a distribution of electron velocities; the glow discharge and considers the cold cathode and hot cathode discharge phenomena; ionization by electron collision, electron attachment, ion mobility, ion–ion and electron–ion recombination, and other important processes that affect the conduction of electricity in gases; illustrates the importance of gaseous electronics with several important phenomena and technical applications.

88 Applications to Combustion

David R. Crosley

There have been two major advances in combustion research: the use of powerful computers for the numerical solutions to combustion problems, and the use of laser diagnostic techniques for the determination of the detailed properties of the combustion system. This chapter concentrates on these two areas of physical models and laser diagnostics, and the outstanding physical question that remain. Each is greatly influencing the development of the two important combustion science issues: describing turbulent flows and incorporating realistic chemistry.

89 Surface Physics

Erik T. Jensen

This chapter describes various applications of atomic and molecular physics to phenomena that occur at surfaces. Particular attention is placed on the application of electron- and photon–atom scattering processes to obtain surface specific structural and spectroscopic information.

90 Interface with Nuclear Physics

John D. Morgan III, James S. Cohen

The effect of finite nuclear size on the electronic energy levels of atoms is presented; and conversely, the electronic structure effects in nuclear physics are discussed. The chapter ends with an analysis of muon-catalyzed fusion.

91 Charged Particle–Matter Interactions

Hans Bichsel

In the description of the interaction of fast charged particles with matter, two aspects can be distinguished: the effects on the particle, usually energy losses and deflections, and the spatial distribution of the energy lost by the particle in the absorber. This chapter discusses concepts needed in the operation of charged particle detectors and in describing radiation effects, specifically those used for the instantaneous observation of the passage of a charge particle. Delayed effects are not discussed. The description is restricted to fast charged particles. Energy loss straggling, rather than stopping powers, is primarily considered.

92 Radiation Physics

Mitio Inokuti

Radiation physics entails studies of the interactions of ionizing radiation with matter. This subject is studied to properly build radiation detectors, understand dosimetry, perform risk estimates of exposure to natural and artificial radiation sources, and many others. This chapter concerns key topics in basic radiation physics selected from a vast range of possibilities. The treatment concentrates on basics and principles, and illustrative examples are given.



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