

Preface

The aim of this book is to present the results of calculations of cross-sections and probabilities of a large variety of atomic processes with participation of photons and electrons, namely on photoabsorption, electron scattering, and accompanying effects. Thus, we intend to produce and present newly obtained and previously collected Atomic Data.

Atomic Data are required in a number of scientific domains connected to investigation of electronic structure and physical processes in solids and liquids, molecules and clusters, astronomical objects, solar and planet atmospheres, atomic nucleus, and so on. Deep understanding of chemical reactions and processes is impossible without clear, deep, and accurate knowledge of atomic structure and processes with participation of atoms.

One should not forget also that all atoms except hydrogen and, perhaps, helium, are relatively complex systems by themselves. They are still objects of intensive theoretical and experimental studies, in which sophisticated methods are applied. For planning corresponding experiments and for estimating the value of very sophisticated new theoretical approaches, one needs data that are reasonably accurate, sufficiently general, and relatively easy to obtain. Our book serves this aim.

The role, played by atoms in macrophysics, chemistry, biology, some domains of engineering, and the entire macroworld, is similar to the role played by elementary particles in microworld. Indeed, atoms are the bricks, the main building elements from which the macroscopic world is constructed. The “glue” that keeps together the macroscopic bodies is the interatomic interaction that is modified to some extent, in many cases considerably, when many atoms are bound together.

In spite of obvious demand, there is no such a book available. Usually, if it is a book on experiment, the main focus is on the results of measurements, which are compared with available theoretical results. If a book is on theory, it concentrates on details of the presented theoretical approaches, illustrating their achievements by comparing with experimental data. In both types of books, the main interest is information on considered physical process. Our aim is to concentrate on the calculation data itself. To obtain the data, we will use theoretical methods, which open the possibility of extensive calculations and at the same time are as accurate

as possible. Of course, it would be best of all to have simple analytic formulas to calculate all necessary atomic characteristics and probabilities. Alas, the atomic structure is complicated enough. So, the analytical formulae are too crude. On the other hand, rapid development of computing facilities, PC in particular, permits to perform relatively accurate calculations, using rather complicated theoretical approaches. The result of such an approach is the subject of our book. Main attention will be given to presenting the results of calculations. As to the theoretical methods employed, they will be described briefly in order to clarify how the presented results are obtained.

We will present in this book results obtained in the best one-electron Hartree–Fock (HF) approximation and with account of multielectron correlations in the frame of so-called random phase approximation with exchange-RPAE. The corrections due to the latter proved to be very important in a broad variety of atomic characteristics and processes. There are cases when corrections determined by the multielectron nature of an atom are not too strong but still important. In these cases, we will use also so-called many-body perturbation theory—MBPT.

To explain theoretical consideration and make them as transparent as possible, we will use the diagrammatical technique, or Feynman diagram language of the many-body theory, which will make the consideration of different processes and effects transparent enough. Proper references will advice the potential reader where he or she can find all required details of the theoretical approaches used in this book.

There exist several review papers and books where table of atomic data are presented. But attention was given only to the characteristics of atomic structure, such as total energy of atoms, mean radiuses, and energy of occupied levels. To large extent the level and scope of these calculations were determined not only by the demand of the corresponding data, but also by the technical ability to perform corresponding calculations. Perhaps the first in this direction was the book written by Herman and Skillman [1]. Then several other publications appeared [2–4] where atomic data are tabulated with step by step increasing quality of the data.

In [5] and [6], the data on photoionization cross-sections and dipole angular anisotropy parameter for many atoms are presented. But the calculation results were obtained in the frame of a one-electron approach that is much simpler than HF. It is known, however, that even HF as a rule is very far from being sufficient in describing the experimental photoionization cross-sections for outer and intermediate subshells, as well as near threshold regions of the inner shells. There the role of many-electron correlations is very big. This shortcoming of [5] and [6] is eliminated in this book.

We will not limit our consideration to atoms but investigate also some negative and positive ions. Recently great attention has been given to such atom-like objects as fullerenes and endohedrals—atoms “caged” inside a fullerene shell. As a fullerene we will consider C_{60} and take into account two of its action. The first is the scattering of electrons—incoming and originating from the caged atom. The second is the modification of the incoming photon beam due to C_{60} polarization. Corresponding data will be presented for a number of endohedral atoms and ions.

As it is seen from the title, we will concentrate on the processes of electron and photon interaction with atoms. An essential reason for this is that these processes can be treated theoretically with very high accuracy and reliability. Theoretical description of each considered process will be limited by mentioning the main physical ideas essential for understanding this particular process and some key formulas that are used in our calculations. Only main points of the calculation procedure will be presented.

Such a book, as we do believe, will be important for many specialists and students, both graduate and undergraduate, who have an intention to specialize in atomic physics and related areas. This book will be useful for theorists, performing research in different domains of contemporary physics, chemistry, and biology, for technologists working on production of new materials, and for experimentalists performing research in the field of photon and electron interaction with atoms, molecules, solid bodies, and liquids. On the whole, we strongly believe that there exists a broad audience of potential readers for such a book. This is confirmed by multitude of references to our predecessors [1.1–1.6].

We will show that the data collected and the method used in obtaining these data can be useful in the theoretical description of the experiments, which are already performed. Moreover, the data can be very effective in suggesting new experiments, creating a number of desirable imaginable experiments, for which theoretical estimations or even calculations can be performed beforehand. All this could help experimentalists to plan their activity more effectively by performing preliminary rather simple investigation and research that is meaningful to call theoretical experiment.

On the whole, we will consider in this book many different physical processes, almost everything connected to the interaction of atoms and ions with photons, electrons, and positrons. For each of these processes, we will present results in one-electron Hartree–Fock approximation and with account of multielectron correlations in the frame of either the random phase approximation with exchange (RPAE) or many-body perturbation theory (MBPT).

As reference books on Quantum Mechanics and Electrodynamics in their description of atomic structure and processes, we will use the following two: Landau LD, Lifshitz EM (1977) *Quantum mechanics: non-relativistic theory*, 3rd edn. Pergamon Press and Berestetskii VB, Lifshitz EM, Pitaevskii LP (1982) *Quantum electrodynamics*, 2nd edn. Butterworth-Heinemann, Oxford. In calculating atomic characteristics and scattering cross-sections, usually radial, angular, and spin variables are separated and the integration over the angular variables and summation over spin projections are performed analytically. As a reference guide for these operations we use the book of Sobelman II (1972) *Introduction to the theory of atomic spectra*. Elsevier. The references to all these sources will be given as [LL], [BLP], and [IS].

Considerable overlap, particularly noticeable in notations, diagrams, which represent the physical processes, and the presentation of mathematical formulas used in this book, exists with previous publications: Amusia MYa, *Atomic photoeffect*. Plenum Press, New York and Amusia MYa, Chernysheva LV (1997) *Computation*

of atomic processes. Institute of Physics Publishing, Bristol. The references to them will be given as [AM] and [AC]. Theoretical formalism, essential for the topic of this book, can be found also in a recent book: Amusia MYa, Ivanov VK, Cherepkov NA, Chernysheva LV (2006) Processes in many-electron atoms. Nauka, Saint Petersburg, pp 1–325 (in Russian). The reference to it will be given as [AICC].

Throughout this book, we will use the atomic system of units, setting Planck's constant \hbar , electron charge e , and its mass m equal to 1, since otherwise formulae, calculations, and expressions will be overloaded by powers of \hbar , m , and e . If another system of units, with $e = 1.6 \times 10^{-19}$ C and $m = 9,108 \times 10^{-31}$ kg is used, the following are the atomic units: length $a_0 = \hbar^2/me^2 = 0.529 \times 10^{-10}$ m = 5.29×10^{-1} nm; energy $\varepsilon_0 = 2 \text{ Ry} = me^4/\hbar^2 \approx 27.21$ eV = 43.59×10^{-10} nJ; cross-section $a_0^2 \approx 27.98 \times 10^{-18}$ cm² = $27.98 \times 10^{-4}(\text{nm})^2 = 27.98$ Mb (1 Mb being equal to 10^{-18} cm²); velocity $v_0 = (e_0/m)^{1/2} = e^2/\hbar \approx 2.188 \times 10^6$ m/s; and time $t_0 = a_0/v_0 = \hbar^3/me^4 \approx 0.242 \times 10^{-16}$ s. Units of angular momentum are \hbar and $\hbar/a_0 = me^2/\hbar$. The fine structure constant is $\alpha = e^2/\hbar c \approx 1/137.04$. In the atomic system $\alpha = 1/c$ and the speed of light is $c \approx 137.04$.

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