
SPECTROSCOPIC CONSTANTS OF ATOMS AND IONS

Spectra of Atoms with
One or Two Electrons

V. A. Boyko V. G. Pal'chikov I. Yu. Skobelev A. Ya. Faenov

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PREFACE

The beginning of the twentieth century, which brought us the basic theory of the structure of matter or quantum mechanics, has also moved atomic spectroscopy to the position of one of the leading fields of physics. Spectroscopic experiments have been one of the best tests of this theory. In the course of birth and development of various physical concepts, spectroscopy turned into the most powerful method of study of the structure of matter and has made its way into many scientific and practical applications.

During recent years the spectroscopy of atoms and ions in the visible, ultra-violet, and soft X-ray range has become very popular due to intense development of thermonuclear fusion, laser science, and accelerator technology. The reason is that besides providing essential information about atom and ion structure, atomic spectroscopy is capable of developing methods of measuring the parameters of a substance subjected to extreme conditions (super-high temperatures and pressures), solving problems of preservation of measurement uniformity, and improving the uniform system of standards and units of physical quantities in quantum metrology (a new field of metrology). The development of metrology in this particular direction is guided by the application of new physical principles for search and utilization of stable quantum effects in order to improve precision of measurements, to determine values of the fundamental constants, and to improve the system of standards and highly precise measurement methods.

The system of modern diagnostic methods which has been developed on the basis of the spectroscopy of atoms and ions requires first of all reliable and precise data concerning the most basic spectroscopic constants of atomic systems, i.e., the ionization potential, structure of energy levels, and radiative transition probabilities.

Presently this type of experimental information exists not only for neutral atoms but also for multiply-charged ions, whose spectral lines are located within a previously little-studied X-ray wavelength of $\lambda = 0.1$ to 1 nanometers. Simultaneously with the above-mentioned, an intense development of new methods in relativistic theory and employment of new fast computers have provided a significant amount of fairly precise theoretical data (at least for systems with a small number of electrons). However, the existing theoretical and experimental data on spectra of atoms and ions are spread through a large number of periodicals, which makes it difficult to utilize this information for practical spectroscopy.

In this book the authors systematically try to present the results of experimental and theoretical studies of spectra of the simplest atomic systems containing one or two electrons (atoms of hydrogen and helium, as well as ions of their isoelectronic sequences) and to provide a systemized set of reference data about their spectroscopic characteristics. On the one hand, the above-mentioned information has the highest precision and reliability, whereas on the other hand, it is necessary for the development of spectral diagnostic techniques to identify complex atomic spectra and develop methods for the calculation of structures of multielectron atoms and ions.

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1.1. Retrospective Review of Experimental Studies

The first studies of the spectral series of HI and HeII were conducted in the last century. The spectra of hydrogen-like ions with $Z \geq 3$ nuclear charges were observed for the first time by Adlen and Erickson in the 1930s, whereas the spectra for those ions where $Z \geq 6$ were observed somewhat later. Presently there are experimental data on hydrogen-like ions with $Z = 1, \dots, 18, 20, 22, 24, 26, 28, 29, 36,$ and 42 [1].

The HI spectrum is most thoroughly studied. Besides the Lyman series, by the end of the 1950s data had been obtained on 42 lines of the Balmer series, 5 lines of the Brackett series, 2 lines of the Pfund series, and the principal line of the sixth series. Somewhat later Hansen and Strong discovered the principal line of the seventh series. In the 1960s and 1970s radio frequency methods were applied for a detailed study of the fine structure of the levels with $n \leq 5$, where n is the principal quantum number, and the fine structure of the main line of the Balmer series was resolved for the first time. The most precise measurements of the $2s-3p$ transition (the relative error is $\Delta\lambda/\lambda \approx 10^{-9}$ are presented in reference [2], which presently provides the most precise experimental value of the Rydberg constant — $R_\infty = 109737.31521(11) \text{ cm}^{-1}$.

The spectrum of the HeII singly-charged ion has been studied to a similar extent. In the works published by the end of the 1960s and the beginning of the 1970s, scientists measured values of the fine-structure splitting (including the Lamb shift) with $n \leq 6$, and resolved the fine structure of a number of lines of the Paschen and Brackett series.

Much less studied are the spectra of multiply-charged hydrogen-like ions ($Z \geq 3$). It is worth noting here both Adlen and Tyren's works, as well as a number of studies conducted relatively recently, starting at the end of the 1960s.

Experimental values of the Lamb shift $2s_{1/2}-2p_{1/2}$ are presently known for ions LiIII, Cvi, Qvii, Fix, Pxxv, Clxvii, and Arxviii. Their measurement error is between $5 \cdot 10^{-3}$ and $1 \cdot 10^{-2}$, and ordinarily it rises with increase of the ionic charge. Experiments now being planned [3] should improve the precision of the Lamb shift to the range 10^{-4} to 10^{-3} at $Z \approx 10$.

A significant amount of data concerning the spectra of hydrogen-like ions. Bv, Cvi, Nvii, Oviii, Fix, Nex, Sixiv, and Clxvii was obtained by the end of the 1970s by means of the beam-foil method. The spectral resolution and measurement precision of the wavelengths in these experiments were relatively low (the most common measurement error is ± 0.2 nanometer for $\lambda > 50$ nanometers and ± 0.5 nanometer for $\lambda < 20$ nanometers), although, for example, the application of the laser resonance method reference [4] has enabled measurement of 9–10 transition wavelengths in the Fix ions

with $\Delta\lambda/\lambda = 5 \cdot 10^{-5}$. Nowadays, the precision of measurement of beam-foil experiments has improved and, for example, in reference [5] the first 6 lines of the Lyman series of FeX and SiXIV ions were measured with relative error of $5 \cdot 10^{-4}$ to 10^{-3} . Approximately similar precision has been achieved during studies of the spectra of ions CVI, OVIII, and FeX in a laser plasma.

The laser plasma technique was used for obtaining the X-ray spectrum of hydrogen-like ions NaX through SXVI [6]. The spectra of the more highly-charged ions (ArXVIII, TiXXII, CrXXIV, FeXXNi, NiXXVIII, CuXXIX, and MoXLII) were recorded in a low pressure linear discharge, in a low induction vacuum spark, in the plasma focus. As far as the above-mentioned ions are involved, there are only experimental data practically speaking on the first several lines of the Lyman series. The error of the wavelengths for these lines is sufficiently small ($\approx 5 \cdot 10^{-4}$ to 10^{-3} ; nevertheless it is higher than the uncertainty of the theoretical calculation. Approximately the same error appears in measurements of the wavelengths of hydrogen-like ions which are present in the plasma of the solar corona. In recent work on the spectra of multiply-charged ions in the Tokamak [7], as well as during the beam-foil excitation [8, 9], the transition energy Ly_{α} in ions ArXVIII, and FeXXVI has been measured with high precision (the error is $\approx 10^{-4}$).

1.2. Theory of Spectra of Hydrogen-Like Ions

The problem of specification of the theory of spectra of hydrogen-like ions has recently acquired greater importance due to numerous metrological studies of these atomic systems. Presently this chapter of the theory is probably the most fully developed area for the application of both quantum mechanics and quantum electrodynamics, and it provides a basis for the development of the theory of multielectron atomic systems. The development of modern quantum-field methods and new methods of numerical processing on powerful computers have significantly advanced the theory in this particular direction.

The main task of the theoretical description of spectra of multiply-charged ions lies first of all in calculations of wavelengths, the intensity of spectral lines, the probabilities of radiative and autoionizing transitions. Although these problems are common to atomic spectroscopy as a whole, the use of thoroughly developed methods of calculation of neutral atoms is not entirely satisfactory because of the increasing importance of relativistic and quantum-electrodynamic effects. The manifestation of these effects appears, for example, in an increase of intensity of the spectral lines which are forbidden by the selection rules, an increase of ionization potentials up to several hundreds or even thousands of electron volts, in a shift of spectra to the vacuum ultra-violet and X-ray range.

Until recently the principal source of information on transition wavelengths in hydrogen-like ions was the design data published in reference [10]. In the above-mentioned work the energy levels were calculated on the basis of the precisely solved Dirac equation with the following consideration of corrections linked both to the nuclear structure and quantum-electrodynamic effects. Since then the precision of the fundamental constants and the relevant theoretical calculations have increased drastically. The most complete analysis of modern achievements of quantum electrodynamics in the area

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APPENDIX

This section presents the experimental values of energies and transition wavelengths in the spectra of hydrogen- and helium-like ions which have been published in recent years, but were not included in the Russian edition of the book. The experimental data presented in the appendix have been compared with the theoretical calculations conducted by quantum electrodynamics. The values of the fundamental physical constants, $R_\infty = 109737.31534(13) \text{ cm}^{-1}$ and $\alpha^{-1} = 137.0359895(61)$, recommended by the CODATA group [60] differ slightly from those in the book, $R_\infty = 109737.31521(11) \text{ cm}^{-1}$ and $\alpha^{-1} = 137.035965(12)$. However, these differences have no practical influence on the tabular data compiled in the book. An exception are the energy levels of atomic hydrogen and the He^+ ion. Even here, however, in most cases the difference affects only the last significant digit or is within the error limits of the theoretical calculation. On the other hand, the precision of the calculations of energy levels and transition wavelengths for these atoms (except the Lamb shift) significantly exceeds the accuracy of presently existing experimental observation.

The tables in the Appendix are as follows:

1. Table 4.1. Comparison between theoretical calculations and observed data of the Lamb shift in hydrogen like ions
2. Table 4.2. Comparison between theoretical calculations and observed wavelengths of Lyman transitions in hydrogenlike ions
3. Table 4.3. $1snp \ ^1P_1$ energies of the ^4He atom
4. Table 4.4 Observed wavelengths of $1s \ ^2S_0 - 1snp \ ^1P_1$ transitions in the ^4He atom
5. Table 4.5. Observed transition energies in the ^4He atom
6. Table 4.6. Observed wavelengths for the $2^3S_1 - 2^3P_2$ transition
7. Table 4.7. Observed wavelengths for the $2^3S_1 - 2^3P_0$ transition
8. Table 4.8. Observed wavelengths for the $2^3S_1 - 2^3P_1$ transition
9. Table 4.9. Comparison between observed and theoretical wavelengths of the $1 \ ^1S_0 - 2 \ ^3S_1$ and $1 \ ^1S_0 - n \ ^1,3P_j$ transitions in multiply charged heliumlike ions