МІНІСТЕРСТВО ОСВІТИ І НАУКИ УКРАЇНИ
ОДЕСЬКИЙ ДЕРЖАВНИЙ ЕКОЛОГІЧНИЙ УНІВЕРСИТЕТ

Methodical instructions for practical work, test performance, distance learning of PhD students in the discipline "Atomic Optics and Spectroscopy", Part 7 (Training of PhD students of the specialty: 104 –"Physics and astronomy")

«Затверджено»
на засіданні групи забезпечення спеціальності
Протокол №1 від 28/08/2021 Голова групи_____Свинаренко А.А.

«Затверджено»
на засіданні кафедри вищої та прикладної математики
Протокол №1 від 28/08/2021 Зав. кафедри_____Глушков О.В.

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Methodical instructions for practical work, test performance, distance learning of PhD students in the discipline "Atomic Optics and Spectroscopy", Part 7 (Training of PhD students of the specialty: 104 –"Physics and astronomy")

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Methodical instructions for practical work, test performance, distance learning of PhD students in the discipline “Atomic Optics and Spectroscopy”, Part 7. (Training specialty: 104 - “Physics and Astronomy”; 01.04.05- “Optics and Laser Physics” and others)

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PREFACE

Discipline "Atomic optics and spectroscopy" is a compulsory discipline in the cycle of professional training of postgraduate students (3 level of education) in specialty 104 – Physics and Astronomy (specialization: 01.04.05 -optics and laser physics). **It is aimed at** assimilating (assuring) a number of planned competences, including the study of the modern apparatus of Atomic optics and spectroscopy, as well as the development of new computational methods of determination and treating spectra of diatomic and multiatomic molecules, their energetic and spectroscopic characteristics on the basis of methods of quantum mechanics and quantum electrodynamics, the ability to analyze data of numerical experiments on the study of Atomic energetic, optical, spectroscopic characteristics that can be large and require the use of powerful computing resources, the use of modern existing and new advanced methods in order to achieve scientific results that create potentially new knowledge in Atomic optics and spectroscopy.

The place of discipline in the structural-logical scheme of its teaching: the knowledge gained during the study of this discipline is used in the writing of dissertations, the topics of which are related to determination and treating spectra of diatomic and multiatomic molecules, their energetic and spectroscopic characteristics on the basis of methods of quantum mechanics and quantum electrodynamics. **The basic concepts** of discipline are the fundamental tools of a specialist in the field of Physics and Astronomy (specialization: 01.04.05 - optics and laser physics).

The purpose of studying the discipline is assimilation (assurance) of a number of competencies, in particular, the achievement of the relevant knowledge, understanding and the ability to use the advanced methods of Atomic optics and spectroscopy, as well as the development of new computational methods of determination and treating spectra of diatomic and multiatomic molecules, their energetic and spectroscopic characteristics on the basis of methods of quantum mechanics and quantum electrodynamics, to the needs of the dissertation before - study, adapt, improve quantum (Atomic) methods to analyze data on Atomic spectra, results of numerical experiments on the study of Atomic energetic, optical, spectroscopic characteristics.

After mastering this discipline, the postgraduate student must be able to use modern or personally developed new methods, in particular, to analyze, simulate, predict, and program the spectra of diatomic and multiatomic molecules. These methodical instructions are for self-studying work of the second-year PhD students and tests performance in the discipline «Atomic optics and spectroscopy».

Topics: Spectra of lanthanide and actinide atoms. Influence of relativistic effects (spin-orbit interaction) on the structure and intensity of spectral lines

Topics: Spectra of lanthanide and actinide atoms. Influence of relativistic effects (spin-orbit interaction) on the structure and intensity of spectral lines
Топіки: Спектри атомів лантанідів та актинідів. Вплив релятивістських ефектів (спін-орбітальної взаємодії) на структуру та інтенсивність спектральних ліній (ЗБ- Л2.10)

1. Introduction

Theoretical studying spectrum of the excited states for the ytterbium atom is carried out within the relativistic many-body perturbation theory with ab initio zeroth approximation and generalized relativistic energy approach. The zeroth approximation of the relativistic perturbation theory is provided by the optimized Dirac-Kohn-Sham ones. Optimization has been fulfilled by means of introduction of the parameter to the Kohn-Sham exchange potentials and further minimization of the gauge-non-invariant contributions into radiation width of atomic levels with using relativistic orbital set, generated by the corresponding zeroth approximation Hamiltonian. The obtained theoretical data on energies E and widths W of the ytterbium excited states are compared with alternative theoretical results (the Dirac-Fock, relativistic Hartree-Fock, perturbation theories) and available experimental data. Analysis shows that the theoretical and experimental values of energies are in good agreement with each other, however, the values of widths differ significantly. In our opinion, this fact is explained by insufficiently accurate estimates of the radial integrals, the use of unoptimized bases, and some other approximations of the calculation.

A great interest in the study of radiation and autoionization processes involving electrons, photons, atoms and ions is stimulated by new classes of problems, in particular, in modern laser physics and physics of astrophysical, thermonuclear, laser and other plasmas (see [1-52]). In recent years, among atomic systems, special attention has been paid to the experimental and theoretical study of the spectral characteristics of heavy atoms, including atoms of lanthanides and actinides, as well as multiply charged ions. Traditionally, they are used in astrophysical research, in studies of the physics of laboratory plasma generated by various sources: laser pulses, tokamaks, pinches, capillary discharges, etc., in studies of thermonuclear fusion. For several decades,

methods for the experimental study of the spectroscopic characteristics of the radiation of multiply charged ions have been developed and improved. A detailed description of experimental techniques can be found in a number of well-known books, reviews, and original experimental works (see, e.g., [1-52]).
A modern quantum mechanics of atoms (as well as molecules) has undergone significant development over the past few decades. It is possible to recall such well-known, along with those mentioned above, methods such as the Rayleigh-Schrödinger, Möller-Plesset perturbation theory (PT) method, PT in 1/Z parameter (Z is the charge of the atomic nucleus) and electron-electron interaction, PT with a model potential approximation, with Hartree-Fock (HF) or Dirac-Fock (DF) zeroth approximations andd many others. The multi-configuration DF method is the most reliable version of calculation for multielectron systems with a large nuclear charge. One should remember about very complicated structure of spectra of the heavy atoms, including actinides, uranium, trans-uranium elements and others and necessity of correct accounting for the different correlation effects such as polarization interaction of the valent quasiparticles and their mutual screening, iterations of a mass operator etc.).

The aim of our present work is to use an effective method of relativistic many-body PT with an optimized ab initio Dirac-Kohn-Sham approximation [27-30] to study spectrum of excited states for the ytterbium.

2. The relativistic many-body perturbation theory and energy approach

As the method of computing is earlier presented in detail, here we are limited only by the key topics [27-30]. According to these Refs., the majority of complex atomic systems possess a dense energy spectrum of interacting states with essentially relativistic properties. In the theory of the non-relativistic atom a convenient field procedure is known for calculating the energy shifts ΔE of degenerate states. This procedure is connected with the secular matrix M diagonalization [30-32]. In constructing M, the Gell-Mann and Low adiabatic formula for ΔE is used.

In contrast to the non-relativistic case, the secular matrix elements are already complex in the second order of the electrodynamical PT (first order of the interelectron interaction). Their imaginary part of ΔE is connected with the

radiation decay (radiation) possibility. In this approach, the whole calculation of the energies and decay probabilities of a non-degenerate excited state is reduced to the calculation and diagonalization of the complex matrix *M*. In the papers of different authors, the $\mathrm{Re}\Delta E$ calculation procedure has been generalized for the case of nearly degenerate states, whose levels form a more or less compact group. One of these variants has been previously introduced: for a system with a dense energy spectrum, a group of nearly degenerate states is extracted and their matrix *M* is calculated and diagonalized. If the states are well separated in energy, the matrix *M* reduces to one term, equal to ΔE. The non-relativistic secular matrix elements are expanded in a PT series for the interelectron interaction. The complex secular matrix *M* is represented in the form [26,27]:

$$M = M^{(0)} + M^{(1)} + M^{(2)} + M^{(3)}. \quad (1)$$

where $M^{(0)}$ is the contribution of the vacuum diagrams of all order of PT, and $M^{(1)}$, $M^{(2)}, M^{(3)}$ those of the one-, two- and three- quasiparticle diagrams respectively. $M^{(0)}$ is a real matrix, proportional to the unit matrix. It determines only the general level shift. We have assumed $M^{(0)} = 0.$ The diagonal matrix $M^{(1)}$ can be presented as a sum of the independent one-quasiparticle contributions. For simple systems (such as alkali atoms and ions) the one-quasiparticle energies can be taken from the experiment. Substituting these quantities into (1) one could have summarized all the contributions of the one -quasiparticle diagrams of all orders of the formally exact QED PT. However, the necessary experimental quantities are not often available.

The first two order corrections to $\mathrm{Re}M^{(2)}$ have been analyzed previously using Feynman diagrams (look Ref. in [2,3]). The contributions of the first-order diagrams have been completely calculated. In the second order, there are two kinds of diagrams: polarization and ladder ones. The polarization diagrams take into account the quasiparticle interaction through the polarizable core, and the ladder diagrams account for the immediate quasiparticle interaction [30-36]. Some of the ladder diagram contributions as well as some of the three-quasiparticle diagram contributions in all PT orders have the same angular symmetry as the two-quasiparticle diagram contributions of the first order.

These contributions have been summarized by a modification of the central potential, which must now include the screening (anti-screening) of the core potential of each particle by the two others. The additional potential modifies the one-quasiparticle orbitals and energies.

Then the secular matrix is as follows:

$$M \to \tilde{M}^{(1)} + \tilde{M}^{(2)}, \qquad (2)$$

where $\tilde{M}^{(1)}$ is the modified one-quasiparticle matrix (diagonal), and $\tilde{M}^{(2)}$ the modified two-quasiparticle one. $\tilde{M}^{(1)}$ is calculated by substituting the modified one-quasiparticle energies), and $\tilde{M}^{(2)}$ by means of the first PT order formulae for $M^{(2)}$, putting the modified radial functions of the one-quasiparticle states in the radial integrals..

Let us remind that in the QED theory, the photon propagator D(12) plays the role of this interaction. Naturally the analytical form of D(12) depends on the gauge, in which the electrodynamical potentials are written. Interelectron interaction operator with accounting for Breit interaction has been taken as follows:

$$V\left(r_i r_j\right) = exp\left(i\omega r_{ij}\right) \cdot \frac{\left(1 - \alpha_i \alpha_j\right)}{r_{ij}}, \qquad (3)$$

where, as usually, α_i are the Dirac matrices. In general, the results of all approximate calculations depended on the gauge. Naturally the correct result must be gauge-invariant. The gauge dependence of the amplitudes of the photoprocesses in the approximate calculations is a known fact and is investigated by Grant, Armstrong, Aymar and Luc-Koenig, Glushkov-Ivanov-Ivanova et al (see review in [9,32]). Grant has investigated the gauge connection with the limiting non-relativistic form of the transition operator and has formulated the conditions for approximate functions of the states, in which the amplitudes of the photo processes are gauge invariant (see review in [9]). These results remain true in the energy approach because the final formulae for the probabilities coincide in both approaches. Glushkov-Ivanov have developed a new relativistic gauge-conserved version of the energy approach [32]. In ref. [27,30,35-40] it has been developed its further generalization. Here we applied

this approach for generating the optimized relativistic orbitals basis in the zeroth approximation of the many-body PT. Optimization has been fulfilled by means of introduction of the parameter to the Fock and Kohn-Sham exchange potentials and further minimization of the gauge-non-invariant contributions into radiation width of atomic levels with using relativistic orbital bases, generated by the corresponding zeroth approximation Hamiltonians [26]. Other details can be found in Refs. [9,27-29,41-47].

3. Some illustrative results and conclusion

Table 1 shows the experimental and theoretical data for the energies (measured from the energy of the ground state: $4f^{14}6s^2\ {}^1S_0$) of some YbI singly excited states [2-7, 28-30]: MCHF-BP - data obtained on the basis of the multi-configuration Hartree-Fock method (MCHF) taking into account Breit-Pauli corrections (BP) (C, D different sets of configurations included in the calculation by the MCHF-BP method [4]); RHF — Cowen data, RHF method; RMBPT (E1) - data of Ivanov-Letokhov et al., Method - relativistic TV with zero approximation MF; data of DF analysis of Wyart-Camus with empirical fit, data of QED-PT [28-30].

Analysis of the data in Table 1 shows that the role of exchange-correlation effects for the studied atom is extremely significant; The HF method with a small number of considered configurations has an error of more than 100 cm-1. Table 2 shows the experimental and theoretical data of Letokhov et al. [17, 82] for the energy and width of excited (autoionization) states of the 7s6p configuration in the YbI spectrum (which originate from the ground state: $4f^{14}6s^2\ {}^1S_0$ Yb): E1, W1 - RMBPT - data of Ivanov et al. [7]; E2, W2 – QED theory [8] (QED-PT); E3-MCHF-BP data from Karacoban-Özdemir [4] (classification in [4] differs from our classification). E4W4 – our data.

Analysis shows that the values of E1-E3, Eexp are in good agreement with each other, however, the values of W1-4, Wexp differ significantly. In our opinion, this fact is explained by insufficiently accurate estimates of the radial integrals, the use of unoptimized bases, and some other approximations of the calculation. This also applies to data obtained from the MCHF and RHF methods.

Table1.

Energy of the ground state: $4f^{14}6s^2\ ^1S_0$) of some YbI singly excited states: MCHF-BP - data obtained on the basis of the multi-configuration Hartree-Fock method (MCHF) taking into account Breit-Pauli corrections (BP) (C, D different sets of configurations included in the calculation by the MCHF-BP method [4]); RHF — the data by Cowan, RHF method; RMBPT - data of Ivanov-Letokhov et al., Method of the relativistic PT with model zeroth approximation; DF-data of DF analysis of Wyart-Camus with empirical fit, QED-PT data, obtained within the relativistic (QED) theory [28-30].

Config.	J	MCHF BPC	MCHF+ BPD	HFR	DF
$6s_{1/2}^{2\,*}$	0	0	0	0	0
$6s_{1/2}6p_{1/2}$	0	17262	18730	17320	17312
$6s_{1/2}6p_{1/2}$	1	17568	18813	17954	17962
$6s_{1/2}6p_{3/2}$	1	26667	25257	25069	25075
$6s_{1/2}6p_{3/2}$	2	18249	18999	19710	19716
$6s_{1/2}5d_{3/2}$	1	28871	23740	24489	24489
$6s_{1/2}5d_{3/2}$	2	28973	24172	24484	24751
$6s_{1/2}5d_{5/2}$	2	29633	26841	27677	27654
$6s_{1/2}5d_{5/2}$	3	29374	25500	25271	25270
Config.	J	QED-PT	RMBPT	Our data	Exp
$6s_{1/2}^{2\,*}$	0	0	0	0	0
$6s_{1/2}6p_{1/2}$	0	17310	17400	17305	17288
$6s_{1/2}6p_{1/2}$	1	18008	18100	18006	17992
$6s_{1/2}6p_{3/2}$	1	25094	25500	25088	25068
$6s_{1/2}6p_{3/2}$	2	19715	19800	19740	19710
$6s_{1/2}5d_{3/2}$	1	24410	23900	24527	24489
$6s_{1/2}5d_{3/2}$	2	24824	24600	24801	24752
$6s_{1/2}5d_{5/2}$	2	26970	26100	26712	27678
$6s_{1/2}5d_{5/2}$	3	25098	24900	25310	25271

Note: * [34] E=-148710cm^{-1}; $E1$=-148700cm^{-1}; $E2$=-148695cm^{-1};

In our calculation, we used an optimized basis of the orbitals of the basis states and more accurately took into account important many-particle exchange-correlation effects, including the polarization and screening interactions of quasiparticles above the closed shells core, the pressure of the continuum and some other effects.

Table 2.

Widths W (cm^{-1}) of autoionization resonances of the YbI 7s6p configuration (see text)

Term	W3	W1	W2	W4	W_{exp}
$^3P_0^0$	-	0.7	1.15	1.12	1.1
$^3P_1^0$	-	3.0	1.10	0.98	0.95
$^3P_2^0$	-	0.7	1.51	1.58	1.6
$^1P_1^0$	-	1.8	2.48	2.55	2.6

To conclude, Theoretical studying spectrum of the excited states for the ytterbium atom is carried out within the relativistic many-body perturbation theory with ab initio zeroth approximation and generalized relativistic energy approach. The zeroth approximation of the relativistic perturbation theory is provided by the optimized Dirac-Kohn-Sham ones. Optimization has been fulfilled by means of introduction of the parameter to the Kohn-Sham exchange potentials and further minimization of the gauge-non-invariant contributions into radiation width of atomic levels with using relativistic orbital set, generated by the corresponding zeroth approximation Hamiltonian. The obtained theoretical data on energies E and widths W of the ytterbium excited states are compared with alternative theoretical results (the Dirac-Fock, relativistic Hartree-Fock, perturbation theories) and available experimental data. Analysis shows that the theoretical and experimental values of energies are in good agreement with each other, however, the values of widths differ significantly. In our opinion, this fact is explained by insufficiently accurate estimates of the radial integrals, the use of unoptimized bases, and some other approximations of the calculation.

Tests performance

Test Option 1.

1). Give the key features of Spectra of lanthanide and actinide atoms. Explain an influence of relativistic effects (spin-orbit interaction) on the structure and intensity of spectral lines: i) mathematical and physical essense of an influence of relativistic effects (spin-orbit interaction) on the structure and intensity of spectral lines; ii) calculation and interpratation of Spectra of lanthanide and actinide atoms, iii) calculation of the relativistic and exchange-correlation contributions into Spectra of lanthanide and actinide atoms v) the technical details of the computation code.

2). Explain all fundamental features of energy and spectroscopic characteristics of lanthanide and actinide atoms, preliminarily describing the corresponding spectra.

3). Perform its pracrical comnputational realization (using Fortran Power Station , Version 4.0; PC Code: “Superatom” for Spectra of lanthanide and actinide atoms **on example of the La** (all necessary numerical parameters should be self-taken).

Test Option 2.

1). Give the key features of Spectra of lanthanide and actinide atoms. Explain an influence of relativistic effects (spin-orbit interaction) on the structure and intensity of spectral lines: i) mathematical and physical essense of an influence of relativistic effects (spin-orbit interaction) on the structure and intensity of spectral lines; ii) calculation and interpratation of Spectra of lanthanide and actinide atoms, iii) calculation of the relativistic and exchange-correlation contributions into Spectra of lanthanide and actinide atoms v) the technical details of the computation code.

2). Explain all fundamental features of energy and spectroscopic characteristics of lanthanide and actinide atoms, preliminarily describing the corresponding spectra.

3). Perform its pracrical comnputational realization (using Fortran Power Station , Version 4.0; PC Code: “Superatom” for Spectra of lanthanide and actinide atoms **on example of the Ce** (all necessary numerical parameters should be self-taken).

Test Option 3.

1). Give the key features of Spectra of lanthanide and actinide atoms. Explain an influence of relativistic effects (spin-orbit interaction) on the structure and intensity of spectral lines: i) mathematical and physical essense of an influence of relativistic effects (spin-orbit interaction) on the structure and intensity of spectral lines; ii) calculation and interpratation of Spectra of lanthanide and actinide atoms, iii) calculation of the relativistic and exchange-correlation contributions into Spectra of lanthanide and actinide atoms v) the technical details of the computation code.

2). Explain all fundamental features of energy and spectroscopic characteristics of lanthanide and actinide atoms, preliminarily describing the corresponding spectra.

3). Perform its pracrical comnputational realization (using Fortran Power Station , Version 4.0; PC Code: "Superatom" for Spectra of lanthanide and actinide atoms **on example of the Pr** (all necessary numerical parameters should be self-taken).

Test Option 4.

1). Give the key features of Spectra of lanthanide and actinide atoms. Explain an influence of relativistic effects (spin-orbit interaction) on the structure and intensity of spectral lines: i) mathematical and physical essense of an influence of relativistic effects (spin-orbit interaction) on the structure and intensity of spectral lines; ii) calculation and interpratation of Spectra of lanthanide and actinide atoms, iii) calculation of the relativistic and exchange-correlation contributions into Spectra of lanthanide and actinide atoms v) the technical details of the computation code.

2). Explain all fundamental features of energy and spectroscopic characteristics of lanthanide and actinide atoms, preliminarily describing the corresponding spectra.

3). Perform its pracrical comnputational realization (using Fortran Power Station , Version 4.0; PC Code: "Superatom" for Spectra of lanthanide and actinide atoms **on example of the Sm** (all necessary numerical parameters should be self-taken).

Test Option 5.

1). Give the key features of Spectra of lanthanide and actinide atoms. Explain an influence of relativistic effects (spin-orbit interaction) on the structure and intensity of spectral lines: i) mathematical and physical essense of an influence of relativistic effects (spin-orbit interaction) on the structure and intensity of spectral lines; ii) calculation and interpratation of Spectra of lanthanide and actinide atoms, iii) calculation of the relativistic and exchange-correlation contributions into Spectra of lanthanide and actinide atoms v) the technical details of the computation code.

2). Explain all fundamental features of energy and spectroscopic characteristics of lanthanide and actinide atoms, preliminarily describing the corresponding spectra.

3). Perform its pracrical comnputational realization (using Fortran Power Station , Version 4.0; PC Code: "Superatom" for Spectra of lanthanide and actinide atoms **on example of the Eu** (all necessary numerical parameters should be self-taken).

Test Option 6.

1). Give the key features of Spectra of lanthanide and actinide atoms. Explain an influence of relativistic effects (spin-orbit interaction) on the structure and intensity of spectral lines: i) mathematical and physical essense of an influence of relativistic effects (spin-orbit interaction) on the structure and intensity of spectral lines; ii) calculation and interpratation of Spectra of lanthanide and actinide atoms, iii) calculation of the relativistic and exchange-correlation contributions into Spectra of lanthanide and actinide atoms v) the technical details of the computation code.

2). Explain all fundamental features of energy and spectroscopic characteristics of lanthanide and actinide atoms, preliminarily describing the corresponding spectra.

3). Perform its pracrical comnputational realization (using Fortran Power Station , Version 4.0; PC Code: "Superatom" for Spectra of lanthanide and actinide atoms **on example of the Er** (all necessary numerical parameters should be elf-taken).

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Methodical instructions
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