We are IntechOpen, the world's leading publisher of Open Access books Built by scientists, for scientists

6,900
Open access books available

185,000
International authors and editors

200M
Downloads

154
Countries delivered to

Our authors are among the
TOP 1%
most cited scientists

12.2%
Contributors from top 500 universities

BOOK CITATION INDEX
CLARIVATE ANALYTICS
INDEXED

WEB OF SCIENCE™

Selection of our books indexed in the Book Citation Index
in Web of Science™ Core Collection (BKCI)

Interested in publishing with us?
Contact book.department@intechopen.com

Numbers displayed above are based on latest data collected.
For more information visit www.intechopen.com

Theoretical Spectroscopy of Rare-Earth Elements: Spectra and Autoionization Resonances

Andrey A. Svinarenko, Alexander V. Glushkov,

Olga Yu. Khetselius, Valentin B. Ternovsky,

Yuliya V. Dubrovskaya, Anna A. Kuznetsova and

Vasily V. Buyadzhi

Additional information is available at the end of the chapter

Abstract

An investigation of spectra, radiative and autoionization characteristics for the rare-earth elements is of a great interest as for development atomic spectroscopy as different applications in plasma chemistry, astrophysics, laser physics, quantum electronics etc. We present and review the results of studying spectra and autoionization resonance characteristics of a few lanthanide elements (ytterbium and thulium). Computing the spectra and autoionization resonance parameters is carried out within the relativistic many-body perturbation theory (RMBPT) and generalized relativistic energy approach. The accurate results on the autoionization resonance energies and widths are presented with correct accounting for the exchange-correlation and relativistic corrections and compared with other available theoretical and experimental data. In this chapter, we present a brief review of the theoretical and experimental works on spectroscopy of some lanthanide atoms. Spectroscopy of the Rydberg autoionization resonances in rare-earth atoms in an external electromagnetic field is expected to be very complex and unusual.

Keywords: rare-earth elements, spectroscopy, relativistic many-body perturbation theory, spectra, autoionization resonances

1. Introduction

An investigation of spectra, optical and spectral, radiative and autoionization characteristics for the rare-earth elements (REEs) (isotopes) and corresponding ions is traditionally of a great

interest due to the further development of quantum optics and atomic spectroscopy and their different applications in the plasma chemistry, astrophysics, laser physics, quantum and nanoelectronics, etc. (see Refs. [1–8]). As it was indicated in many information sources on the rare-earth elements, they make possible the high-tech world—everything from the miniaturization of electronics, to the enabling of green energy and medical technologies, to supporting a myriad of essential telecommunications and defence systems [1, 2]. Besides, it is worth to mention that such industrial operations such as mining, refining and recycling of rare earths can have serious environmental consequences in a case of the improper operations and management. As it was indicated in Ref. [1, 2] that the rare-earth elements all tend to occur together in the same mineral deposits with radioactive elements, particularly thorium and uranium, and because they have similar properties, it is difficult to separate them from one another. Let us remember that according to the modern IUPAC definition, the rare-earth element (REE) is one of a set of 17 chemical elements in the Mendeleev's periodic table, specifically the 15 lanthanides, as well as scandium and yttrium.

Below we will present the results of theoretical investigation of a few lanthanide atoms, namely, ytterbium and thulium. The detailed review of studying energetic, spectral and radiative characteristics of these atoms is presented in a number of monographies and articles [11, 14–86]. One should mention the detailed theoretical studying of the lanthanide atoms by Cowan and pioneer studying by King and Meggers et al., who studied atomic spectra of rare-earth elements and reported wavelengths and relative intensities of more than 1600 lines and estimated intensities of more than 1700 lines of Yb I (see [6–9] and references therein). Camus [14] and Wyart and Camus [15] measured more than 70 absorption lines in the ultraviolet region and obtained the even-parity states with $J = 0$ and $J = 2$ belonging to the series $4f^{14}6sns$ ($n = 13–62$), $4f^{14}6snd$ ($n = 11–64$) and $4f^{14}6snd$ ($n = 11–21$). Moreover, these authors fulfilled new additional observations of the neutral ytterbium spectrum in the infrared region and measured the Zeeman resonance parameters in the visible and near ultraviolet regions. In fact, these measurements allow to propose a new classification of the $4f^{14}\,6snl$ Rydberg series in the Yb spectrum. The configurations $4f^{13}6s^26p$ and $4f^{14}6p^2$ have been complete and the lowest levels of $4f^{13}5d^26s$ and $4f^{14}5d6p$ have been recognized, as well as new low members of the Rydberg series. Spector [16] identified the energy levels of $4f^{13}5d6s^2$ and $4f^{13}6s^26p$ configurations. Highly excited levels of the neutral ytterbium have been studied by means of the two-photon and two-step spectroscopy of even spectra [17] and theoretically by means of the multi-channel quantum defect analysis of the f odd- and even-parity spectra [18].

In Ref. [19], it has been used the method of photoionization laser spectroscopy of the ytterbium atoms in the presence of a direct current (DC) electric field on order to study the Yb photoionization near the first ionization threshold. Blondel et al. [19] had recorded a few spectra corresponding to ionization from the levels $4f^{14}6s7s$ $^1S_0$ and $^3S_1$, $4f^{14}6s6p$ $^1P_1^0$ and $4f^{14}6s5d$ $^1D_2$. The first observation of a long Rydberg series due to single excitation from the $4f^{14}$ subshell in Yb I was reported in Ref. [20] and additionally a two-channel multi-channel quantum defect analysis reveals a prominent series perturbation due to coupling with one particular $4f^{14}5dnf$ doubly excited series. Baig et al. [21] have studied the inner shell and double excitation spectrum of ytterbium involving the $4f$ and $6s$ subshells and reported more than 200 new levels. Theoretical analysis allowed to interpreter these lines as the $4f^{14}6s^2$ to $4f^{13}(^2F_{712,512})nd,ng$ inner

shell transitions and the $4f^{14}6s^2$ to $4f^{14}5d(^2D_{312,512})np,nf$ and $4f^{14}6s^2$ to $4f^{14}6p(^2P_{112,312})ns,nd$ doubly excited ones. All the observed levels lie above the first ionization threshold and can be ordered into Rydberg series converging onto six limits. The interchannel interactions between the overlapped series have been parametrized using multi-channel quantum defect theory.

In Ref. [22], Karaçoban and Özdem carried out the total relativistic computing the energies, Landé factors, lifetimes for a group of the excited levels outside the neutral ytterbium core [Xe]. These authors have used the relativistic Hartree-Fock (RHF) method (the Cowan's atomic code) and the multi-configuration Hartree-Fock (MCHF) method with accounting of the relativistic effects within the Breit-Pauli (BP) scheme (the Fischer's atomic code).

Maeda et al. [23] have used a method of optical-microwave double-resonance spectroscopy to study the highly excited Rydberg states of ytterbium. In Refs. [24, 25], the methods of two-photon ionization and three-photon polarization spectroscopy have been applied to studying the autoionization states (ASs) of the ytterbium atom. The ytterbium atom in the $6s^2$ $^1S_0$ ground state was excited to the $6s6p$ $^3P_1$ excited state by a photon with a visible wavelength (555.648 nm), and it was ionized by absorbing an ultraviolet photon with a wavelength of 260–285 nm. The Rydberg and autoionization states of neutral ytterbium are also considered in Ref. [27]. In Ref. [27], the authors reported the results of a reinvestigation of the $6snf$ $^{1,3}F_3$ ($9 < n < 30$), $6snp$ $^1P_1$ ($12 < n < 56$), $6snp$ $^3P_1$ ($12 < n < 21$) and $6snp$ $^3P_2$ ($12 < n < 19$) Yb Rydberg states using a two-colour three-photon resonant excitation technique through the $4f^{14}6s5d$ $^1D_2$ intermediate level. The novelty of this studying is in the identification of the new levels in the vicinity of the $6snf$ ($9 < n < 16$) Rydberg levels.

The laser spectroscopy method has been effectively applied by Letokhov [28, 29] and Letokhov and co-workers [30, 31] to studying narrow doubly excited autoionization states of ytterbium and other lanthanide atoms. An analysis is made of doubly excited autoionization states of an atom with two valence electrons. The results of experimental and theoretical investigations of narrow autoionization states are reported for ytterbium atoms near the ionization threshold. The method of multi-stage photoionization of atoms by tunable laser radiation was used to detect experimentally and identify narrow autoionization states $^1P_1^0$ and $^3P_{0,1,2}^0$ of the $7s6p$ configuration. In Refs. [32–48], it has been performed the detailed computing energies and widths of the autoionization resonances, Rydberg levels for ytterbium and thallium. The positions and widths of the autoionization states belonging to the $7s6p$, $6p5d$, $6p^2$ and $5d^2$ configurations were calculated using the method of relativistic perturbation theory (PT) with the model potential (MP) zeroth approximation [49–79]. In Refs. [63–68, 85, 86], it has been discovered a principally new spectroscopic effect of a giant broadening autoionization resonances of the lanthanide atoms (thulium and gadolinium) in a sufficiently weak external electric (laser) field. This new effect is of a great importance for problem of laser separation of heavy isotopes and nuclear isomers, spectroscopy and photo-chemistry [65, 66, 93, 94]. It is worth to note from theoretical viewpoint that computing spectra, radiative transition and autoionization parameters of the rare-earth elements' energy is very complicated task because of the necessity of the correct accounting for the exchange-correlation (including polarization and screening effects, a continuum pressure, etc.) and relativistic corrections (and also radiative and nuclear effects in a case of the super heavy

atomic systems). Moreover, theoretical study of spectral properties of the lanthanide atoms is of a great importance for the development of new methods of atomic spectroscopy.

Let us remind that many different quantum-mechanical approaches in the on-relativistic and relativistic versions have been used in order to study energetic and spectroscopic parameters of the lanthanide elements. One should mention such known methods as a standard multi-configuration Hartree-Fock (HP) method with accounting of the relativistic effects within the Breit-Pauli scheme or the classical relativistic Hartree-Fock method or, at last, a multi-configuration Dirac-Fock method. These methods allow to obtain very useful spectral data about many light and heavy atoms. Nevertheless, studying the autoionization resonance characteristics for heavy elements with using the mentioned methods not always provides a precise description of the corresponding spectra. From the other side, at present time, the advanced versions of these methods have been developed, where the one- and two-particle relativistic and exchange-correlation effects are taken into account very precisely. It is worth to remind about computer codes for relativistic many-body calculations of atomic (molecular) properties developed in the Oxford group, Russian-German one, etc. ('GRASP', 'Dirac'; 'BERTHA', 'QED'; see Refs. [1–13] and references therein).

In Refs. [71–88], it has been developed a new formalism of the relativistic many-body PT with using the optimized one-quasiparticle (QP) representation and effective account of the exchange-correlation corrections of the PT second order and higher orders (polarization inter-action, quasiparticles screening, etc.). The method of the relativistic many-body PT is cons-tructed on the basis of the same ideas as the well-known PT with the model potential zeroth approximation by Ivanov et al. [49–64]. However, there are two key differences: namely, the PT zeroth approximation [81, 82, 85, 86] is in fact the Dirac-Kohn-Sham one. In order to calculate the radiative transition and autoionization resonance parameters, a new version of relativistic energy approach is used. It is important to remind that a model relativistic energy approach in a case of the multi-electron atom has been proposed by Ivanov et al. [49–56]. A generalized gauge-invariant relativistic energy approach in a case of the multi-electron atomic systems has been developed by Glushkov-Ivanov-Ivanova (see Refs. [71–76]). It should be noted that an energy approach uses the known Gell-Mann and Low S-matrix scheme. More exactly, a probability of any atomic state radiative decay is connected with an imaginary part of an electron energy shift ΔE, which can be expressed through the Quantum electrodynamics (QED) scattering matrix (by means of the Gell-Mann and Low formula), including the interac-tion with the photon vacuum field (the spontaneous radiative decays) as an external electro-magnetic field (the induced decays) [67–75, 85, 86, 91 92]. In Refs. [71–76], the new energy approach has been combined with a formalism of the relativistic many-body perturbation theory (RMBPT) with an optimized one-quasiparticle representation and an accurate account-ing of the multi-electron exchange-correlation effects.

In this chapter, we present the results of application the optimized relativistic many-body PT with the Dirac-Kohn-Sham zeroth approximation and a generalized relativistic energy approach to studying spectra, radiative and autoionization resonance characteristics for lan-thanide atoms, in particular, ytterbium and thulium. Data on the autoionization resonance energies and widths in the ytterbium and thulium are obtained with correct accounting for the

exchange-correlation and relativistic corrections and compared with other available theoretical and experimental data.

2. Method of relativistic many-body perturbation theory and relativistic energy approach

As our method of computing has been in detail presented previously, here we summarize only the key points. Generally speaking, the energy spectra for the majority of complex atomic systems (naturally including the rare-earth elements) are characterized by a great density. Moreover, these spectra have essentially relativistic properties. So, a correct theoretical method of their studying can be based on the convenient field procedure, which includes computing the energy shifts ΔE of the degenerate electron states. More exactly, speech is about constructing secular matrix M (with using the Gell-Mann and Low adiabatic formula for ΔE), which is already complex in the relativistic theory, and its further diagonalization [49, 50, 55, 56]. In result, one could compute the energies and decay probabilities of a non-degenerate excited state for a complex atomic system [49–64]. The secular matrix elements can be further expanded into a PT series on the interelectron interaction. Here, the standard Feynman diagrammatic technique is usually used.

Generally speaking, the secular matrix M can be represented as follows:

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

where $M^{(0)}$ is the contribution of the vacuum diagrams of all PT orders (this contribution determines only the general levels spectrum shift); $M^{(1)}$, $M^{(2)}$ and $M^{(3)}$ are contributions of the 1-, 2- and 3-quasiparticle (QP) diagrams, respectively. The matrix $M^{(1)}$ can be presented as a sum of the independent one-QP contributions. Substituting these quantities into Eq. (1) one could have summarized all the one-QP diagram contributions. In the empirical methods here, one could use the experimental values of one-electron energies; however, the necessary experimental quantities (especially for the rare-earth and other elements) are not often available. The detailed procedure for computing Re $M^{(2)}$ is presented, for example, in Refs. [51–56].

We will describe an atomic multi-electron system by the relativistic Dirac Hamiltonian (the atomic units are used) as follows [17, 18]:

$$H = \sum_i \{\alpha c p_i - \beta c^2 - Z/r_i\} + \sum_{i>j} \exp(i|\omega|r_{ij})(1 - \alpha_i \alpha_j)/r_{ij} \tag{2}$$

where Z is a charge of nucleus, α_i and α_j are the Dirac matrices, ω_{ij} is the transition frequency, c is the velocity of light. The interelectron interaction potential (the second term in Eq. (3)) takes into account the retarding effect and magnetic interaction in the lowest order on the parameter of the fine structure constant. In the PT zeroth approximation, it is used ab initio mean-field potential:

$$V^{DKS}(r) = [V^D_{Coul}(r) + V_X(r) + V_C(r|b)] \tag{3}$$

with the standard Coulomb, exchange Kohn-Sham V_X and correlation Lundqvist-Gunnarsson Vc potentials (see details in Refs. [75–79]). An effective approach to accounting the multi-electron polarization contributions is described earlier and based on using the effective two-QP polarizable operator, which is included into the PT first-order matrix elements.

In order to calculate the radiation decay probabilities and autoionization energies and widths, a gauge invariant relativistic energy approach (version [71–76]) is used. In particular, a width of the state, connected with autoionization decay, is determined by coupling with the continuum states and calculated as square of the matrix element [73–76]:

$$
\begin{aligned}
V_{\beta_1\beta_2;\beta_4\beta_3} &= \sqrt{(2j_1+1)(2j_2+1)(2j_3+1)(2j_4+1)}(-1)^{j_1+j_2+j_3+j_4+m_1+m_2} \\
&\times \sum_{a\mu}(-1)^{\mu} \begin{pmatrix} j_1 & j_3 & a \\ m_1 - m_3 & \mu \end{pmatrix} \begin{pmatrix} j_2 & j_4 & a \\ m_2 - m_4 & \mu \end{pmatrix} \times Q_a(n_1l_1j_1n_2l_2j_2; n_4l_4j_4n_3l_3j_3)
\end{aligned}
\tag{4}
$$

Here $Q_a = Q_a^{Qul} + Q_a^{Br}$, where Q_a^{Qul} and Q_a^{Br} correspond to the Coulomb and Breit parts of the relativistic interelectron potential in Eq. (3) and express through Slater-like radial integrals and standard angle coefficients. Other details can be found in Refs. [71–92].

The most complicated problem of the relativistic PT computing the rare-earth element spectra is in an accurate, precise accounting for the multi-electron exchange-correlation effects (including polarization and screening effects, a continuum pressure, etc.), which can be treated as the effects of the PT second and higher orders. Using the standard Feynman diagrammatic technique, one should consider two kinds of diagrams (the polarization and ladder ones), which describe the polarization and screening exchange-correlation effects. The detailed description of the polarization diagrams and the corresponding analytical expressions for matrix elements of the polarization QPs interaction (through the polarizable core) potential is presented in Refs. [51–56]. An effective approach to accounting of the polarization diagram contributions is in adding the effective two-QP polarizable operator into the PT first-order matrix elements. In Refs. [55, 56], the corresponding non-relativistic polarization functional has been derived. More correct relativistic expression has been presented in Refs. [11, 81, 82] and used in our computing. The corresponding polarization potential looks as follows [81, 82]:

$$
\begin{aligned}
V^d_{pol}(r_1r_2) = X \left\{ \int \frac{dr' \left(\rho_c^{(0)}(r')\right)^{1/3}\theta(r')}{|r_1 - r'| \cdot |r' - r_2|} \right. \\
\left. - \int \frac{dr' \left(\rho_c^{(0)}(r')\right)^{1/3}\theta(r')}{|r_1 - r'|} \int \frac{dr'' \left(\rho_c^{(0)}(r'')\right)^{1/3}\theta(r'')}{|r'' - r_2|} \Bigg/ \left\langle \left(\rho_c^{(0)}\right)^{1/3} \right\rangle \right\}
\end{aligned}
\tag{5a}
$$

$$\left\langle \left(\rho_c^{(0)}\right)^{1/3} \right\rangle = \int dr \left(\rho_c^{(0)}(r)\right)^{1/3}\theta(r), \tag{5b}$$

$$\theta(r) = \left\{ 1 + [3\pi^2 \cdot \rho_c^{(0)}(r)]^{2/3}/c^2 \right\}^{1/2} \tag{5c}$$

where ρ_c^0 is the core electron density (without account for the quasiparticle), X is numerical coefficient and c is the light velocity. The contribution of the ladder diagrams (these diagrams describe the immediate QPs interaction) is summarized by a modification of the PT zeroth approximation mean-field central potential (see below), which include the screening (anti-screening) of the core potential of each particle by the two others. The details of this contribution can be found in Refs. [71–92]. All computing were performed with using the modified PC code 'Superatom-ISAN'.

3. Spectra and autoionization state characteristics for the ytterbium and thulium atoms

3.1. Spectroscopy of excited and autoionization states in ytterbium

The Yb ($Z = 70$) atom has the external electron configuration $4f^{14}6s^2$ in the ground state and any excited states of the ytterbium atom can be treated as the states with two- or three quasiparticles above the electron core [Xe]$4f^{14}$. **Figure 1** shows a qualitative spectrum of the ytterbium, according to Ref. [30, 31].

In the Yb spectrum, it is possible to define two main types of the autoionization states (ASs) [28, 29]. The state of the first type arises with the excitation of inner shells, the condition of the second type with the double excitation of the valence shell. Those arising from the excitation of the $4f$-shell belong to the intermediate type. Autoionization decay in single-particle approximation can be represented as follows: $\alpha_1\alpha_2 \rightarrow \alpha_3 k$, where α_i (i = 1, 2, 3) describes the set of quantum numbers of bound states, k is the state of free electron. The decay is possible only in a state of continuum, which matches the original AS by parity and value of a total momentum J.
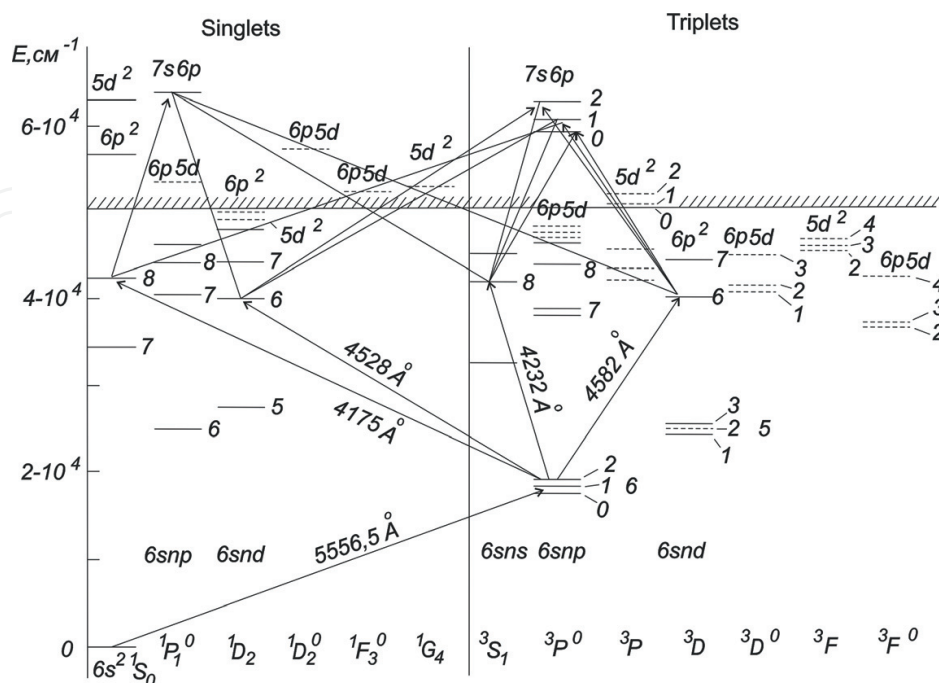

Figure 1. The scheme of energy levels in the Yb spectrum (from Ref. [30, 31]).

Low-lying AS of the Yb atom, arising from the double excitation of $6s^2$ shell, decays under the scheme $n_1l_1n_2l_2 \rightarrow 6skl$. State with electronic configuration $4f^{13}6s^27nl$ is a low-lying auto-ionization state AS with excitation of electron-hole type. The energy areas of these states and states with excited $6s^2$-shell match. The decay of such AS takes place under the scheme: $4f^{13}6s^27nl \rightarrow 4f^{14}6skl'$. Wide low-lying AS ($\Gamma \approx 100$ cm^{-1}) observed in the experiment by Letokhov and co-workers [30, 31] are attributed to such states. The estimation of the AS energy with configurations $6p5d$, $6p^2$, $5d^2$, $7s6p$ in one-particle approximation indicates that these states should be located in the area of 0–15,000 cm^{-1} above Yb ionization threshold. As one could see from **Figure 1**, it is clear that in this case, even configurations $6p^2$, $5d^2$ can be excited in two stages, and the odd $6p5d$, $7s6p$ can be excited in three stages. This fact has been used in the experiments by Letokhov and co-workers [30, 31]. In this experiment, the Yb atoms were excited into the AS by radiation of three dye lasers. The laser of the first stage ($\lambda_1 = 5556.5$ Å) excited transition $6s^{21}S_0 \rightarrow 6s6p\ P_1^0$ (see **Figure 1**). The second laser provided the further excitation to the one of selected intermediate states. The wavelength of the third laser was rebuilt in a such range it provided AS excitation in the studied area 0–15,000 cm^{-1} above the ionization threshold. In particular, upon AS excitation through $6s6d^1D_2$ state the wavelength of the third stage varied in the range 7100–4100 Å, which allowed to ionize Yb atoms, excited in $^1D_2$ state and carry out search of AS in the area of 3700–14,000 cm^{-1}. **Figure 2** shows the dependence of ion current on the third stage laser wavelength, under excitation of the AS $7s6p$ $^3P0^0$ from the $6s6d^3D_1$ state by laser radiation with the line width of ~1 cm^{-1}. **Figure 2** also shows the AS $^3P0^0$ with the width of the laser line of the three stage ~0.1 cm^{-1}.

In **Table 1**, we present the experimental [51, 54] and theoretical data for the energy (energy count from ground state $4f^{14}6s^2\ ^1S_0$) of some YbI singly excited states: MCHF-BP, data obtained on the basis of multi-configuration Hartree-Fock (MCHF) method with Breit-Pauli (BP) adjustments (A, B + D, D different sets of configurations included in the calculation by the method MCHF-BP [22]); RHF—the relativistic Hartree-Fock data [1, 2]; DF—analysis of Wyart-Camus
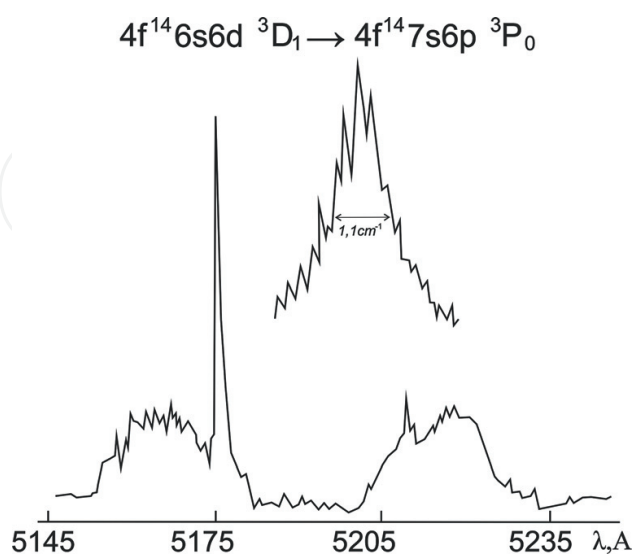

$$4f^{14}6s6d\ ^3D_1 \rightarrow 4f^{14}7s6p\ ^3P_0$$

1,1cm^{-1}

5145   5175   5205   5235 λ,A

Figure 2. Dependence of ion current on the third stage laser wavelength, under excitation of the AS $7s6p\ ^3P0^0$ from the $6s6d^3D_1$ state by laser radiation with the line width of ~1 cm^{-1}.

Config.	J	MCHF + BP(A)	MCHF + BP(C)	MCHF + BP(BD)	RHF	RPTMP	Our theory	DF	Exp
$6s_{1/2}^{2*}$	0	0	0	0	0	0	0	0	0
$6s_{1/2}6p_{1/2}$	0	18,087	17,262	18,730	17,320	17,400	17,310	17,312	17,288
$6s_{1/2}6p_{1/2}$	1	18,174	17,568	18,813	17,954	18,100	18,008	17,962	17,992
$6s_{1/2}6p_{3/2}$	1	24,614	26,667	25,257	25,069	25,500	25,094	25,075	25,068
$6s_{1/2}6p_{3/2}$	2	18,357	18,249	18,999	19,710	19,800	19,715	19,716	19,710
$6s_{1/2}5d_{3/2}$	1	24,094	28,871	23,740	24,489	23,900	24,410	24,489	24,489
$6s_{1/2}5d_{3/2}$	2	24,505	28,973	24,172	24,484	24,600	24,824	24,751	24,752
$6s_{1/2}5d_{5/2}$	2	26,984	29,633	26,841	27,677	26,100	26,970	27,654	27,678
$6s_{1/2}5d_{5/2}$	3	25,860	29,374	25,500	25,271	24,900	25,098	25,270	25,271

* E = −14,8710 cm^{-1}; E1 = −148,700 cm^{-1}; E2 = −148,695 cm^{-1} [45–48].

Table 1. Energies (cm^{-1}) of YbI singly excited states: MCHF-BP, with Breit-Pauli (BP) adjustments (A, B + D, D, different sets of configurations); RHF, relativistic Hartree-Fock method; RPTMP (E1), relativistic perturbation theory with model potential (MP) zeroth approximation [30, 31]; DF, analysis of Wyart-Camus [15]; RPT-DKS (E2), our theory and experiment data (Exp).

[15]; RPTMP (E1)—relativistic perturbation theory with model potential (MP) zeroth approximation by Ivanov et al. [30, 31]; RPT-DKS (E2)—our theory and experiment data (Exp).

The analysis of the calculated data (**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 gives an error of more than 100 cm^{-1}. In **Table 2**, we list the experimental and theoretical data of Letokhov and co-workers [30, 31] for the energy and width of the excited (AS) states of the $7s6p$ configuration in the YbI spectrum (counted from the ground state $4f^{14}6s^{2}\,{}^{1}S_0$Yb): E1, Γ1—RMBPT data by Ivanov et al. [30, 31]; E2, Γ2—our theory (RPT-DKS); E3—MCHF-BP data by Karacoban-Özdemir [22] (classification in [19] differs from our classification).

The analysis of data in **Table 2** shows that the values E1, E2 and E$_{exp}$ are in good agreement with each other, however, values Γ1 and Γ$_{exp}$ differ significantly. In our opinion, this fact is due to the lack of accurate estimates of the radial integrals, use of non-optimized bases and some other approximations of the calculation. This applies to data obtained on the basis of RHF and MCHF methods. In our calculation, we used optimized one-QP representation and optimal relativistic bases and accounted more accurately for the important multi-particle exchange-correlation effects, including polarization and screened interaction of quasiparticles, continuum

Term	Theory E3	Theory E1	Theory Γ1	Theory E2	Theory Γ2	Exp. E$_{exp}$	Exp. Γ$_{exp}$
${}^{3}P_0{}^{0}$	61,233	59,800	0.7	59,450	1.15	59130.5	1.1
${}^{3}P_1{}^{0}$	62,085	60,000	3.0	60,315	1.10	60428.7	0.95
${}^{3}P_2{}^{0}$	62,423	62,600	0.7	62,587	1.51	62529.1	1.6
${}^{1}P_1{}^{0}$	64,216	63,600	1.8	63,613	2.48	63655.8	2.6

Table 2. Energies E (cm^{-1}) and widths Γ (cm^{-1}) of the autoionization resonances of configuration YbI $7s6p$ (see text).

pressure. In **Table 3**, we list the data on energies (counted from the energy of the ground state Yb $4f^{14}$) excited AS with double excited valence shell: E1—RMBPT data (Ref. [30, 31]), E2—our theory.

In **Tables 4** and **5**, we list the analogous data for energies and widths of the other AS. In whole, analysis of these data shows that the results of our theory and the theory of Ivanov et al. regarding energies are in reasonable agreement with the experimental data.

However, in respect of the AS widths there is a reasonably large discrepancy between the theories, which is associated with the use of different basis of orbitals, different degree of accounting for the correlation effects, including continuum pressure (accounted channels $nln'n'-nl\varepsilon s(p,d,f)$).

Config.	J	E1 Theor.	E2	Exp: E_{exp}
$6p_{1/2}^2$	0	−1067	−1064	−1062.7
$6p_{3/2}^2$	2	−987	−1004	−1008.9
$6p_{1/2}6p_{3/2}$	1	−1054	−1050	−1049
$6p_{1/2}6p_{3/2}$	2	−1032	−1036	−1039.5
$5d_{3/2}^2$	2	−1034	−1032	−1010.76
$5d_{3/2}5d_{5/2}$	2	−994	−995	−994.63
$5d_{3/2}5d_{5/2}$	3	−1030	−1032	−1032.47

Table 3. Energies (10^2 cm^{-1}) of the YbI AS with the double excited valence shell (see text).

Conf.	J	E1	E2	Conf.	J	E1	E2
$6p_{1/2}^2$	0	−1067	−1064	$6p_{3/2}5d_{5/2}$	3	−963	−962
$6p_{3/2}^2$	0	−920	−918	$6p_{3/2}5d_{5/2}$	4	−1062	−1061
$6p_{3/2}^2$	2	−987	−1004	$5d_{3/2}^2$	0	−981	−982
$6p_{1/2}6p_{3/2}$	1	−1054	−1050	$5d_{3/2}^2$	2	−1034	−1032
$6p_{1/2}6p_{3/2}$	2	−1032	−1036	$5d_{5/2}^2$	0	−961	−963
$6p_{1/2}5d_{3/2}$	1	−1077	−1072	$5d_{5/2}^2$	2	−970	−968
$6p_{1/2}5d_{3/2}$	2	−1075	−1069	$5d_{5/2}^2$	4	−861	−859
$6p_{1/2}5d_{5/2}$	2	−1007	−1004	$5d_{3/2}5d_{5/2}$	1	−980	−982
$6p_{1/2}5d_{5/2}$	3	−1119	−1115	$5d_{3/2}5d_{5/2}$	2	−994	−995
$6p_{3/2}5d_{3/2}$	0	−1020	−1017	$5d_{3/2}5d_{5/2}$	3	−1030	−1032
$6p_{3/2}5d_{3/2}$	1	−1014	−1012	$5d_{3/2}5d_{5/2}$	4	−1024	−1026
$6p_{3/2}5d_{3/2}$	2	−914	−913	$7s_{1/2}6p_{1/2}$	0	−889	−886.4
$6p_{3/2}5d_{3/2}$	3	−1039	−1035	$7s_{1/2}6p_{1/2}$	1	−887	−886
$6p_{3/2}5d_{5/2}$	1	−949	−948	$7s_{1/2}6p_{3/2}$	1	−851	−849
$6p_{3/2}5d_{5/2}$	2	−1118	−1116	$7s_{1/2}6p_{3/2}$	2	−861	−860

Table 4. Energies (10^2 cm^{-1}) of the YbI AS with the double excited valence shell (see text).

Conf.	J	Term	$\Gamma 1$	$\Gamma 2$	Conf.	J	Term	$\Gamma 1$	$\Gamma 2$
$6p^2_{3/2}$	0	$^1S_0$	5.4	5.69	$6p_{3/2}5d_{3/2}$	2	$^1D_2{}^0$	0.20	0.52
$6p_{3/2}5d_{5/2}$	1	$^1P_1{}^0$	5.7	5.95	$5d^2_{5/2}$	0	$^1S_0$	3.30	3.63
$6p_{3/2}5d_{5/2}$	3	$^1F_3{}^0$	1.60	1.98	$5d^2_{5/2}$	2	$^3P_2$	0.40	0.73
$5d^2_{3/2}$	0	$^3P_0$	0.01	0.05	$5d^2_{5/2}$	4	$^1G_4$	0.90	1.74
$5d_{3/2}5d_{5/2}$	1	$^3P_1$	–	0.0008					

Table 5. Widths (cm^{-1}) of the YbI AS with the double excited valence shell.

The analysis shows that the state of the $5d_{3/2}5d_{5/2}$ ($J = 1$) having an abnormally small width is AS, due to the fact that its decay is prohibited in the non-relativistic limit. This remarkable fact has been found by Ivanova et al. for the first time. From the numerical viewpoint, this effect can be linked with the presence of multiple oscillations of the wave functions in the electron core area.

On the other hand, we are talking about the phenomenon, inherent in heavy atoms and associated with a complex energetics of their valence shells. This fact in principle largely explains unusual and very rich physics of the AS in the lanthanide (rare-earth) atoms. Furthermore in **Tables 6** and **7**, we list the results of computing the energies and widths of autoionization resonances $4f^{13}$ $[^2F_{7/2}]6s^2np[5/2]_2$, $4f^{13}$ $[^2F_{7/2}]6s^2nf[5/2]_2$, resulting from the excitation of electrons in 4f-shell. For comparison, there is data from experimental measurements via three-photon laser polarization spectroscopy method (see [24, 25] and references therein).

Here, one should pay attention to the smallness of the widths of desired resonances, which has not been explained in the literature in detail. In our opinion, this is due to the complex energetics of the studied atom (heavy multi-electron core), causing some unusual physics of AS and mechanisms of their decay, especially in comparison with the usual standards of

n	E_{exp}	Γ_{exp}	E (our theory)	Γ (our theory)
12	70120.5	1.5	70,121	1.7
13	70482.0	0.4	70,483	0.5
15	70914.8	1.2	70,916	1.4
20	71428.1	0.6	71,429	0.7
25	71612.5	1.3	71,611	1.5
26	71633.3	0.6	71,631	0.8
30	71698.8	0.5	71,697	0.7
31	71710.3	0.4	71,712	0.5
34	–	–	71,741	0.3
35	–	–	71,748	0.5

Table 6. Energies and widths (cm^{-1}) of autoionization resonances $4f^{13}$ $[^2F_{7/2}]6s^2np[5/2]_2$, resulting from the excitation of electrons in 4f-shell.

n	E_{exp}	Γ_{exp}	E (our theory)	Γ (our theory)
12	70963.6	0.5	70,965	0.7
13	71105.0	0.4	71,107	0.5
15	71312.2	1.4	71,313	1.6
20	71559.1	0.8	71,561	0.9
25	71672.5	0.5	71,673	0.8
26	71687.5	0.5	71,689	0.7
30	71732.4	0.4	71,734	0.5
31	71741.2	0.5	71,740	0.6
34	–	–	71,763	0.8
35	–	–	71,770	0.5

Table 7. Energies and widths (cm^{-1}) of autoionization resonances $4f^{13}$ [$^2F_{7/2}$]$6s^2nf$[5/2]$_2$, resulting from the excitation of electrons in $4f$-shell.

atomic spectroscopy (typical AS widths for the He atom, atoms of the inert gases, alkali and alkali-earth atoms reach dozens and hundreds cm^{-1}).

3.2. Spectroscopy of excited and autoionization states in thulium

In contrast to the ytterbium atom, the thulium atom has been studied to a much lesser extent. Moreover, it is not difficult to understand that this atom is theoretically more complex than the ytterbium atom. In Refs. [32–41], it has been shown that two pairs of low-lying ionization limits (with vacancy states in the $4f^{14}$ shell: $4f_{7/2}^{-1}4f_{5/2}^{-1}$; here and below we write $4f_j^{-1}$ instead of $4f_j^{13}$) cause two main types of autoionization decay (**Figure 3**):

1. the classical decay channel of Beutler-Fano (BFD)

$$4f_{5/2}^{-1}6s_{1/2}(J_{12})nl \rightarrow 4f_{7/2}^{-1}6s_{1/2}(J_{12'})\mathrm{Tm}^+ + \varepsilon l_e j_e, n > 7, J_{12} = 2; 3, J_{12'} = 3; 4, \qquad (6)$$

2. the re-orientation-type decay (ROD) channel

$$4f_j^{-1}6s_{1/2}(J_{12})nl \rightarrow 4f_j^{-1}6s_{1/2}(J_{12'})\mathrm{Tm}^+ + \varepsilon l_e j_e, n > 25, J_{12} = 3, J_{12'} = 2; 4, j = 5/2, 7/2 \qquad (7)$$

Here ROD refers to re-orientation-type AS decay. The states $4f_{5/2}^{-1}6s_{1/2}(J_{12} = 3)nl$ are exposed simultaneously to BFD and ROD-decays. In contrast to BFD-decay, ROD-decay is a low energy process, preserving one-electron quantum numbers of the atomic core: $4f_j^{-1}$ and $6s_{1/2}$. The ROD-decay can be of both monopole and quadrupole nature.

This refers to the QPs interaction multi-polarity that causes the AS decay. The states with $J_{12} = 2;4$ are unable to disintegrate through ROD channel. However, their mixing with the states of the
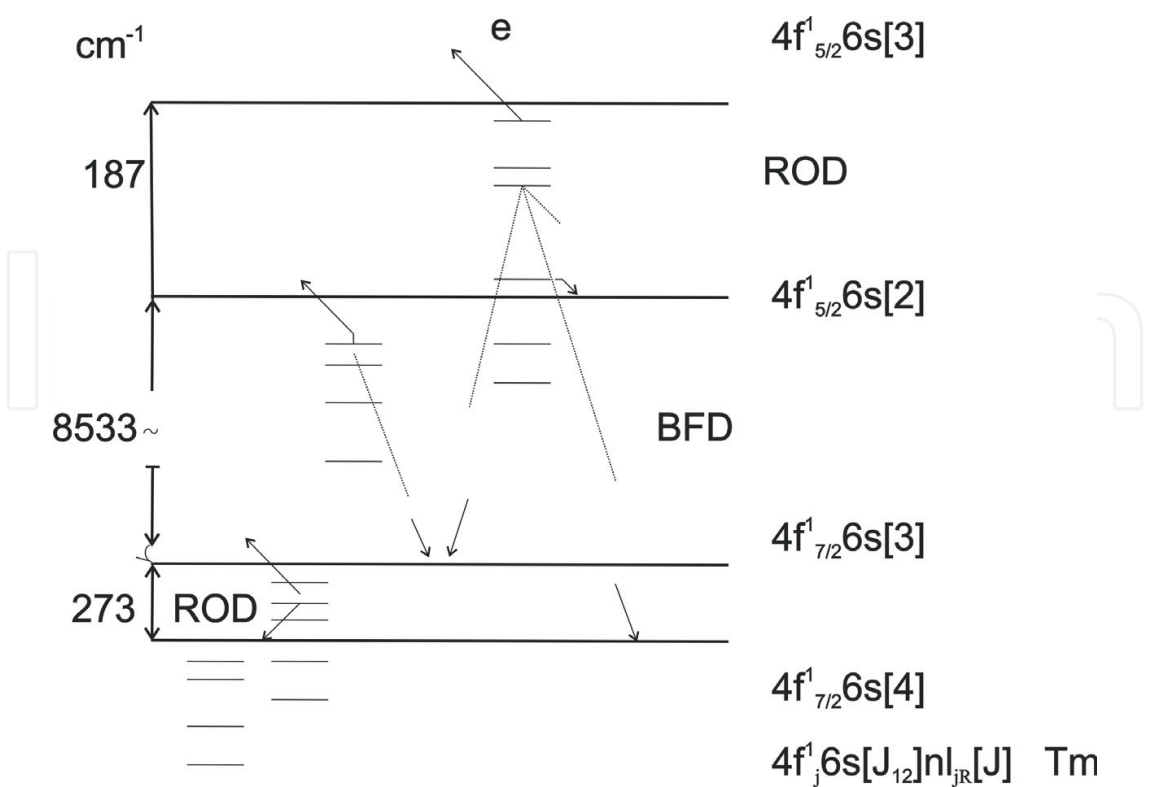
Figure 3. Position of the low-lying Tm atom $4f^16snl$ ionization limits and scheme of autoionization decay of Tm atom Rydberg states $4f^{13}6snl$.

ROD decaying type can greatly improve monopole ROD decay of the latter. For these Rydberg series, there is only possible AS decay channel—re-orientation one ROD. In **Table 8**, we list the results of computing the energies E2 (10 cm^{-1}) and widths Γ2 (cm^{-1}) of the AS $4f^{-1}_j 6s(J_{12})nsnp[J]$ of the Tm atom with $n = 25$–35, namely, the AS $4f^{13}_{7/2}6s_{1/2}(3)ns_{1/2}[J]$, for which the ROD-decay is the only autoionization decay channel. For comparison, we list the calculated data obtained by Ivanov et al. (E1, Γ1) [32–41] and Glushkov et al. (E, Γ3) [6].

In **Tables 9** and **10**, we list our data on the widths and energies of the Tm AS $4f^{13}_{7/2}6s_{1/2}(3)np_j[J]$ and $4f^{13}_{5/2}6s_{1/2}(2)ns_{1/2}[J]$, for which BFD is the only autoionization decay channel. In Table 10,

	J = 5/2			J = 5/2			J = 7/2	J = 7/2
n	Γ1	Γ3	Γ2	E1	E3	E2	Γ2	E2
25	1.18 (−5)	1.29 (−5)	1.25 (−5)	4985	4981	4983	1.58 (−2)	4986
26	–	–	1.13 (−5)	–	–	4975	1.34 (−2)	4988
30	5.77 (−6)	6.72 (−6)	6.12 (−6)	4995	4993	4994	3.98 (−3)	4995
33	–	–	3.79 (−6)	–	–	4996	1.58 (−2)	4998
35	–	–	3.21 (−6)	–	–	4998	3.18 (−3)	5000

Table 8. Widths and energies of the Tm AS $4f^{13}_{7/2}6s_{1/2}(3)ns_{1/2}[J]$.

(j,J)	(3/2, 3/2)		(1/2, 5/2)		(3/2, 5/2)	
n	Γ2	E2	Γ2	E2	Γ2	E2
25	4.68 (−5)	49,862	1.40 (−1)	49,858	1.92 (−1)	49,865
26	4.22 (−5)	49,877	1.33 (−1)	49,874	1.75 (−1)	48,979
30	2.42 (−5)	49,939	1.03 (−1)	49,937	1.07 (−1)	49,941
33	1.80 (−5)	49,971	7.54 (−2)	49,968	8.20 (−2)	49,972
35	1.39 (−5)	49,992	5.72 (−2)	49,990	6.59 (02)	49,993
(j, J)	(1/2, 7/2)		(3/2, 7/2)		(3/2, 9/2)	
n	Γ2	E2	Γ2	E2	Γ2	E2
25	3.72 (−2)	49,848	3.46 (−1)	49,867	3.98 (−1)	49,869
26	3.45 (−2)	49,863	3.24 (−1)	49,884	3.71 (−1)	49,886
30	2.38 (−2)	49,938	2.38 (−1)	49,952	2.62 (−1)	49,953
33	2/12 (−2)	49,961	2.05 (−1)	49,977	2.26 (−1)	49,978
35	1.76 (−2)	49,982	1.56 (−1)	49,992	1.729 (−1)	49,993

Table 9. Widths and energies of the Tm AS $4f_{7/2}^{13}6s_{1/2}(3)np_j[J]$ (our data).

	J = 3/2	J = 3/2	J = 5/2	J = 5/2
n	Γ2	E2	Γ2	E2
25	2.64 (−5)	5836	5.32 (−5)	5838
30	1.27 (−5)	5845	2.78 (−5)	5846
35	8.89 (−6)	5850	1.54 (−5)	5852

Table 10. The widths (cm^{-1}) and energies (10^2 cm^{-1}) of the Tm AS $4f_{5/2}^{13}6s_{1/2}(2)ns_{1/2}[J]$.

we list our data on the widths and energies (in cm^{-1}) of AS $4f_{5/2}^{13}6s_{1/2}(3)ns_{1/2}[J]$, which can decay in both the ROD and the BFD channels.

4. Conclusions

We have presented a brief review of the theoretical and experimental papers on spectroscopy of the rare-earth elements of ytterbium and thulium and some results of theoretical studying their spectra. Computing energy level positions and autoionization resonance widths and energies is fulfilled on the basis of the generalized relativistic energy approach and relativistic many-body PT with the Dirac-Kohn-Sham zeroth approximation and accurate accounting for the exchange-correlation and relativistic corrections. Spectral data for some autoionization resonances, such as the Rydberg ones, or autoionization states with the double excited valence shell and others are of a great interest as they reveal a sufficiently

high complexity of rare-earth elements (in particular, ytterbium and thulium) from the atomic spectroscopic viewpoint, indicating a rather complex dynamics of the decay of such states. Namely, these states play an important role in various atomic elementary processes in plasmas and gases. The Rydberg autoionization states are of considerable interest, for example, for the creation of new types of lasers, studies on the laser separation of heavy isotopes and nuclear isomers and the corresponding applications such as an analysis of trace quantities of rare-earth elements, etc. It should also be noted that the dynamics of the decay of autoionization resonances in ytterbium, thallium and other rare-earth elements in an external electromagnetic (laser) field is expected to be extremely complex and unusual. In any case, further study of the spectra, characteristics of the radiation and autoionization decay of the autoionization states in spectra of the rare-earth atoms is extremely important and actual.

Author details

Andrey A. Svinarenko*, Alexander V. Glushkov, Olga Yu. Khetselius, Valentin B. Ternovsky, Yuliya V. Dubrovskaya, Anna A. Kuznetsova and Vasily V. Buyadzhi

*Address all correspondence to: svinarenkoaa@gmail.com

Odessa State Environmental University, Odessa, Ukraine

References

[1] www.rareelementresources.com/rare-earth-elements

[2] Bourzac K. Can the US Rare-Earth Industry Rebound?. Technology Review. 2010 October

[3] Martin W. NIST Spectra Database, Version 2.0 (http://physics.nist.gov.asd). Washington: NIST; 2004

[4] Cowan RD. The Theory of Atomic Structure Spectra. Berkeley: University of California Press; 1981

[5] Grant IP. Relativistic Quantum Theory of Atoms and Molecules, Theory and Computation. Vol. 40. Berlin: Springer; 2007

[6] Glushkov AV. Relativistic Quantum Theory. Relativistic Quantum Mechanics of Atomic Systems. Odessa: Astroprint; 2008. 700 p

[7] Glushkov AV. Atom in Electromagnetic Field. Kiev: KNT; 2005. 400 p

[8] Khetselius OY. Hyperfine Structure of Atomic Spectra. Odessa: Astroprint; 2008. 208 p

[9] Kohn W, Sham S. Quantum density oscillations in an inhomogeneous electron gas. Physical Review A. 1965;**137**:1697–1710

[10] Safronova UI, Johnson W, Derevianko A. Relativistic many-body calculations of energy levels, hyperfine constants, electric-dipole matrix elements, static polarizabilities for alkali-metal atoms. Physical Review A. 1999;**60**:4476–4486

[11] Khetselius OY, Florko TA, Svinarenko AA, Tkach TB. Radiative and collisional spectroscopy of hyperfine lines of the Li-like heavy ions and Tl atom in an atmosphere of inert gases. Physica Scripta. 2013;**T153**:014037

[12] Khetselius OY. Spectroscopy of cooperative electron-gamma-nuclear processes in heavy atoms: NEET effect. Journal of Physics: Conference Series. 2012;**397**:012012

[13] Dzuba V, Flambaum V, Silvestrov P, Sushkov D. Many-body perturbation theory calculations in atoms with open shells. Physical Review A. 1991;**44**:2828–2831

[14] Camus P, Debarre A, Morillon C. Two-photon absorption spectroscopy in ytterbium. Journal of Physics B: Atomic and Molecular Physics. 1978;**11**:L395–L398

[15] Wyart J-F, Camus P. Extended analysis of the emission spectrum of neutral ytterbium (Yb I). Physica Scripta. 1979;**20**(1):43–52

[16] Spector N. Configurations 4fN–16s26p in neutral gadolinium, dysprosium, erbium, and ytterbium. Journal of the Optical Society of America A. 1971;**61**(10):1350–1354

[17] Camus P, Debarre A, Morillon C. Highly excited levels of neutral ytterbium. I. Two-photon and two-step spectroscopy of even spectra. Journal of Physics B: Atomic and Molecular Physics. 1980;**13**(6):1073–1087

[18] Aymar A, Debarre A, Robaux O. Highly excited levels of neutral ytterbium. II. Multichannel quantum defect analysis of odd- and even-parity spectra. Journal of Physics B: Atomic and Molecular Physics. 1980;**13**:1089–1096

[19] Blondel C, Champeau RJ, Delsart C. Photoionisation laser spectroscopy of ytterbium atoms in the presence of a DC electric field. Journal of Physics B: Atomic and Molecular Physics. 1985;**18**(12):2403–2414

[20] Baig MA, Connerade JP. The interchannel interaction between single excitation from 4f14 and double excitation from 6s2 in Yb I. Journal of Physics B: Atomic and Molecular Physics. 1984;**17**:L469–L474

[21] Baig MA, Ahmad S, Griesmann U, Connerade JP, Bhatti SA, Ahmad N. Inner shell and double excitation spectrum of ytterbium involving the 4f and 6s subshells. Journal of Physics B: Atomic and Molecular Physics. 1992;**25**(2):321–332

[22] Karaçoban B, Özdem L. Energies, landé factors, and lifetimes for some excited levels of neutral Ytterbium (Z = 70). Acta Physica Polonica B. 2011;**119**(3):342–353

[23] Maeda H, Matsuo Y, Takami M, Suzuki A. Optical-microwave double-resonance spectroscopy of highly excited Rydberg states of Yb. Physical Review A. 1992;**45**:1732–1742

[24] Yi J, Lee J, Kong HJ. Autoionization states of the ytterbium atom by three-photon polarization spectroscopy. Physical Review A. 1995;**51**(4):3053–3057

[25] Yi J, Park H, Lee J. Investigation of even parity autoionization states of ytterbium atoms by two-photon ionization spectroscopy. Journal of the Korean Physical Society. 2001;**39** (5):916–920

[26] Xu CB, Xu XY, Huang W, Chen DY. Rydberg and autoionization states of neutral ytterbium. Journal of Physics B: Atomic and Molecular Physics. 1994;**27**(17):3905–3913

[27] Raheel A, Yaseen M, Nadeem A, Bhatti SA, Baig MA. Two-colour three-photon excitation of the 6snf 1,3F3 and 6snp 1P1, 3P1,2 Rydberg levels of YbI. Journal of Physics B: Atomic, Molecular and Optical Physics. 1999;**32**(4):963–965

[28] Letokhov VS. Nonlinear Selective Photoprocesses in Atoms and Molecules. Moscow: Nauka; 1983. 408 p

[29] Bekov GI, Vidolova-Angelova EP, Ivanov LN, Letokhov VS, Mishin VI. Laser spectroscopy of narrow doubly excited autoionization states of ytterbium atoms. Soviet Physics— JETP. 1981;**53**(3):441–447

[30] Vidolova-Angelova EP, Ivanov LN, Letokhov VS. Application of model potential method in calculating Rydberg states of rare-earth elements Tm, Yb, Lu and their ions. Journal of Physics B: Atomic, Molecular and Optical Physics. 1982;**15**(73):981–991

[31] Vidolova-Angelova EP, Ivanov LN, Letokhov VS. Application of model potential method in calculating Rydberg states of rare-earth elements Tm, Yb, Lu and their ions. Journal of Physics B: Atomic, Molecular and Optical Physics. 1984;**17**(6):953–961

[32] Vidolova-Angelova EP, Ivanov LN, Ivanova EP, Angelov DA. Relativistic perturbation method for studying radiation decay of highly-excited many-electron atoms: Tm. Journal of Physics B: Atomic, Molecular and Optical Physics. 1986;**19**:2053–2069

[33] Vidolova-Angelova EP, Ivanov LN, Angelov DA. Autoionization decay of excited Rydberg Tm states. Journal of Physics B: Atomic, Molecular and Optical Physics. 1988;**21**:3877–3890

[34] Vidolova-Angelova EP, Ivanov LN. Autoionization Rydberg states of thulium. Re-orientation decay due to monopole interaction. Journal of Physics B: Atomic, Molecular and Optical Physics. 1991;**24**:4147–4158

[35] Ivanova EP. Energy levels of ions of silver and rhodium isoelectronic sequences with Z < 86. Optics and Spectroscopy. 2007;**103**(5):733–740

[36] Ivanova EP. Spectroscopic constants of VUV laser transitions in ions of the palladium isoelectronic sequence. Optics and Spectroscopy. 2003;**94**(2):151–156

[37] Ivanova EP, Ivanov AL. Theoretical search for optimal pump parameters for observing spontaneous radiation amplification on the lambda=41.8-nm transition of Xe IX in plasma. Quantum Electronics. 2004;**34**(11):1013–1017

[38] Ivanova EP, Ivanov LN, Aglitsky EV. Modern trends in spectroscopy of multi-charged ions. Physics Reports. 1988;**166**(N6):315–390

[39] Ivanov LN, Ivanova EP, Knight LV, Molchanov AG. Spectrum of plasma containing Ne- and Na-like ions: consistent account for Rydberg and autoionizing Rydberg series in balance equations. Physica Scripta. 1996;**53**(6):653–667

[40] Glushkov AV, Khetselius OY, Svinarenko AA. Theoretical spectroscopy of autoionization resonances in spectra of lanthanides atoms. Physica Scripta. 2013;**T153**:014029

[41] Svinarenko AA. Study of spectra for lanthanides atoms with relativistic many-body perturbation theory: Rydberg resonances. Journal of Physics: Conference Series. 2014;**548**:012039

[42] Ivanova EP, Grant IP, Rose SJ. Gain evaluation for the Ni-like tantalum X-ray laser. X-ray Lasers Proc. 1999;383-386

[43] Ivanova EP, Grant IP. Effects of oscillator strength transfer and radiative decay cancellation in Ne-like and Ni-like sequences. Application to X-ray laser modeling and plasma diagnostics. X-ray Lasers Proc. 1999;395-398

[44] Ivanova EP, Ivanov AL, Zinoviev NA, Knight LV. Proposal for X-ray laser pumped by a powerful short-pulse-drive laser. X-ray Lasers Proc. 1999;399-402

[45] Ivanova EP, Ivanov AL, Zinoviev NA, Knight LV. Proposal for the X-ray laser pumped by a powerful short-pulse drive laser. SPIE. 1999;**3735**(1):266–275

[46] Ivanova EP, Zinoviev AN. The possibility of X-ray lasers based on the innershell transitions of Ne-like ions. Physics Letters A. 2000;**274**(5):239–246

[47] Ivanova EP, Zinoviev NA. Time history of gain calculations in radiative-collisional model for X-ray lasers. Journal de Physique IV. 2001;**11**(2):151–154

[48] Ivanova EP, Zinoviev NA, Knight LV. Theoretical investigation of a Ni-like xenon X-ray laser in the 13-14 nm range. Quantum Electronics. 2001;**31**(8):683–688

[49] Ivanov LN, Ivanova EP. Extrapolation of atomic ion energies by model potential method: Na-like spectra. Atomic Data and Nuclear Data Tables. 1979;**24**(2):95–121

[50] Driker MN, Ivanova EP, Ivanov LN, Shestakov AF. Relativistic calculation of spectra of 2-2 transitions in O-and F-like atomic ions. Journal of Quantitative Spectroscopy and Radiative Transfer. 1982;**28**(6):531–535

[51] Ivanov LN, Podobedova LI. Formally exact perturbation theory with a model potential as a zeroth approximation. I. Transition energies in Fe ions including effects of inner-shell electrons. Journal of Physics B: Atomic and Molecular Physics. 1977;**10**(6):1001–1013

[52] Ivanov LN, Safronova UI, Senashenko VS, Viktorov DS. The radiationless decay of excited states of atomic systems with two K-shell vacancies. Journal of Physics B: Atomic and Molecular Physics. 1978;**11**(6):L175–L179

[53] Ivanov LN, Letokhov VS. Selective ionization of atoms in optical and electric fields. Soviet Journal of Quantum Electronics. 1975;**5**(3):329–332

[54] Ivanov LN, Letokhov VS. Spectroscopy of autoionization resonances in heavy elements atoms. Com. Mod. Phys. D.: At. Mol. Phys. 1985;**4**:169–184

[55] Ivanova EP, Ivanov LN, Glushkov AV, Kramida AE. High order corrections in the relativistic perturbation theory with the model zeroth approximation, Mg-like and Ne-like ions. Physica Scripta. 1985;**32**(4):513–522

[56] Ivanova EP, Ivanov LN, Gurchumeliya AD, Tsirekidze MA, Tsirekidze TA. Correlation effects in heavy multi-electron ions represented by 4-4 transitions in the Zn-like isoelectronic sequence. Journal of Physics B: Atomic and Molecular Physics.1985;**18**(8):1467–1482

[57] Ivanova EP, Glushkov AV. Theoretical investigation of spectra of multicharged ions of F-like and Ne-like isoelectronic sequences. Journal of Quantitative Spectroscopy & Radiative Transfer. 1986;**36**(N2):127–145

[58] Ivanova EP, Ivanov AL. A superpowerful source of far-ultraviolet monochromatic radiation. JETP. 2005;**100**(5):844–856

[59] Ivanova EP, Ivanov AL, Pakhomova TE. X-ray laser at 10-15 nm in Pd-like ions Er XXIII-Re XXX. X-ray Lasers Proc. 2007;353-359

[60] Glushkov AV, Svinarenko AA, Khetselius OY, Buyadzhi VV, Florko TA, Shakhman AN. Relativistic quantum chemistry: Advanced approach to construction of the Green's function of the Dirac equation with complex energy and mean-field nuclear potential. In: Nascimento M, Brändas E, Maruani J, Delgado-Barrio G, editors. Frontiers in Quantum Methods and Applications in Chemistry and Physics. Series: Progress in Theoretical Chemistry and Physics. Vol. 29. Berlin: Springer; 2015. pp. 197–218

[61] Glushkov AV, Malinovskaya SV, Gurnitskaya EP, Khetselius OYu, Dubrovskaya YuV. Consistent quantum theory of recoil induced excitation and ionization in atoms during capture of neutron. Journal of Physics: Conference Series. 2006;**35**:425–430

[62] Ivanov LN, Ivanova EP, Knight L. Energy approach to consistent QED theory for calculation of electron-collision strengths. Physical Review A. 1993;**48**(9):4365–4374

[63] Glushkov AV, Ivanov LN, Letokhov VS. Nuclear quantum optics. Preprint of Institute for Spectroscopy of the USSR Academy of Sciences (ISAN), Moscow-Troitsk. 1991;**AS-N4**:1–16

[64] Glushkov AV, Khetselius OY, Loboda AV, Svinarenko AA. QED approach to atoms in a laser field: Multi-photon resonances and above threshold ionization In: Wilson S, Grout PJ. Maruani J, Delgado-Barrio G, Piecuch P, editors. Frontiers in Quantum Systems in Chemistry and Physics. Series: Progress in Theoretical Chemistry and Physics. Vol. 18. Berlin: Springer; 2008. pp. 543–560

[65] Basov NG, Letokhov VS. Optical frequency standards. Soviet Physics Uspekhi. 1969;**11**(12):855–880

[66] Letokhov VS. Laser induced processes in spectroscopy, isotope separation and photochemistry. Soviet Physics Uspekhi. 1986;**29**(1):70–81

[67] Glushkov AV, Ivanov LN. A broadening of the thulium atom autoionization resonances in a weak electric field. Preprint of Institute for Spectroscopy of the USSR Academy of Sciences (ISAN), Moscow-Troitsk. 1992;**AS-N2**:1–10

[68] Glushkov AV, Ivanov LN. Shift and deformation of radiation atomic lines in the laser emission field. Multiphoton processes. Preprint of Institute for Spectroscopy of the USSR Academy of Sciences (ISAN), Moscow-Troitsk. 1992;**AS-N3**:1–12

[69] Glushkov AV, Khetselius OY, Lopatkin YM, Florko TA, Kovalenko OA, Mansarliysky VF. Collisional shift of hyperfine line for rubidium in an atmosphere of the buffer inert gas. Journal of Physics: Conference Series. 2014;**548**:012026

[70] Svinarenko AA, Khetselius OY, Buyadzhi VV, Florko TA, Zaichko PA, Ponomarenko EL. Spectroscopy of Rydberg atoms in a Black-body radiation field: Relativistic theory of excitation and ionization. Journal of Physics: Conference Series. 2014;**548**:012048

[71] Glushkov AV, Ivanov LN, Ivanova EP. Relativistic decay of excited atomic states. Generalized energy approach. In: Autoionization Phenomena in Atoms. Moscow: Moscow University Press; 1986. pp. 58–160

[72] Glushkov AV. Relativistic and correlation effects in spectra of atomic systems. Odessa: Astroprint; 2006. 400 p

[73] Glushkov AV, Ivanov LN. Radiation decay of atomic states: Atomic residue polarization and gauge noninvariant contributions. Physics Letters A. 1992;**170**(1):33–36

[74] Glushkov AV. Negative ions of inert gases. JETP Letters. 1992;**55**(2):97–100

[75] Glushkov AV, Khetselius OYu, Svinarenko AA. Relativistic theory of cooperative muon-gamma-nuclear processes: Negative muon capture and metastable nucleus discharge. In: Hoggan P, Brandas E, Maruani J, Delgado-Barrio G, Piecuch P, editors. Advances in the Theory of Quantum Systems in Chemistry and Physics. Series: Progress in Theoretical Chemistry and Physics. Vol. 22. Berlin: Springer; 2011. pp. 51–70

[76] Glushkov AV. Advanced relativistic energy approach to radiative decay processes in multielectron atoms and multicharged ions. In: Nishikawa K, Maruani J, Brandas E, Delgado-Barrio G, Piecuch P, editors. Quantum Systems in Chemistry and Physics: Progress in Methods and Applications. Series: Progress in Theoretical Chemistry and Physics. Vol. 26. Berlin: Springer; 2012. pp. 231–254

[77] Glushkov AV, Ambrosov SV, Loboda AV, Chernyakova Yu, Svinarenko AA, Khetselius OYu. QED calculation of the superheavy elements ions: Energy levels, radiative corrections and hfs for different nuclear models. Nuclear Physics A: Nuclear and Hadronic Physics. 2004;**734**:21–28

[78] Svinarenko AA, Nikola LV, Prepelitsa GP, Tkach T, Mischenko E. The Auger (autoionization) decay of excited states in spectra of multicharged ions: Relativistic theory. AIP Conference Proceedings. 2010;**1290**:94–98

[79] Glushkov AV, Ambrosov SV, Loboda AV, Gurnitskaya EP, Khetselius OY. QED calcula-
tion of heavy multicharged ions with account for correlation, radiative and nuclear
effects. In: Julien J-P, Maruani J, Mayou D, Wilson S, Delgado-Barrio G, editors. Recent
Advances in Theoretical Physics and Chemistry Systems. Series: Progress in Theoretical
Chemistry and Physics. Vol. 15. Berlin: Springer; 2006. pp. 285–299

[80] Glushkov AV, Khetselius OYu, Gurnitskaya EP, Loboda AV, Florko TA, Sukharev DE,
Lovett L. Gauge-invariant QED perturbation theory approach to calculating nuclear
electric quadrupole moments, hyperfine structure constants for heavy atoms and ions.
In: Wilson S, Grout PJ. Maruani J, Delgado-Barrio G, Piecuch P, editors. Frontiers in
Quantum Systems in Chemistry and Physics. Series: Progress in Theoretical Chemistry
and Physics. Vol. 18. Berlin: Springer; 2008. pp. 507–524

[81] Glushkov AV. Relativistic polarization potential of a many-electron atom. Soviet Physics
Journal. 1990;**33**(1):1–8

[82] Glushkov AV. Correction for exchange and correlation effects in multielectron system
theory. Journal of Structural Chemistry. 1990;**31**(4):529–533

[83] Glushkov AV, Khetselius OYu, Lovett L. Electron-β-nuclear spectroscopy of atoms and
molecules and chemical environment effect on the β-decay parameters. In: Piecuch P,
Maruani J, Delgado-Barrio G, Wilson S, editors. Advances in the Theory of Atomic and
Molecular Systems Dynamics, Spectroscopy, Clusters, and Nanostructures. Series: Pro-
gress in Theoretical Chemistry and Physics. Vol. 20. Berlin: Springer; 2010. pp. 125–152

[84] Glushkov AV, Lovett L, Khetselius OYu, Gurnitskaya EP, Dubrovskaya YuV, Loboda AV.
Generalized multi configuration model of decay of multipole giant resonances applied to
analysis of reaction (μ-n) on the nucleus ^{40}Ca. International Journal of Modern Physics A.
2009;**24:**611–615

[85] Glushkov AV, Ivanov LN. DC strong-field stark-effect: Consistent quantum-mechanical
approach. Journal of Physics B: Atomic, Molecular and Optical Physics. 1993;**26**(16):
L379–L386

[86] Glushkov AV, Ivanov LN. DC Strong Field Stark effect: Consistent quantum mechanical
approach. Preprint of Institute for Spectroscopy of the USSR Academy of Sciences
(ISAN), Moscow-Troitsk. 1992;**AS-N1**:1–16

[87] Glushkov AV, Loboda A, Gurnitskaya E, Svinarenko A. QED theory of radiation emission
and absorption lines for atoms in a strong laser field. Physica Scripta. 2009;**T135**:014022

[88] Khetselius OYu. On possibility of sensing nuclei of the rare isotopes by means of laser
spectroscopy of hyperfine structure. Sensor Electronics and Microsystem Technologies.
2008;**3**:28–33

[89] Glushkov AV, Malinovskaya SV, Chernyakova YG, Svinarenko AA. Cooperative laser-
electron-nuclear processes: QED calculation of electron satellites spectra for multi-charged
ion in laser field. International Journal of Quantum Chemistry. 2004;**99**(5):889–893

[90]   Glushkov AV, Khetselius OY, Malinovskaya SV. Spectroscopy of cooperative laser–electron nuclear effects in multiatomic molecules. Molecular Physics. 2008;**106**(9):1257–1260

[91]   Glushkov AV. Operator perturbation theory for atomic systems in a strong DC electric field. In: Hotokka M, Maruani J, Brandas E, Delgado-Barrio G, editors. Advances in Quantum Methods and Applications in Chemistry, Physics, and Biology. Series: Progress in Theoretical Chemistry and Physics. Vol. 27. Berlin: Springer; 2013. pp. 161–178

[92]   Glushkov AV, Khetselius OYu, Malinovskaya SV. Optics and spectroscopy of cooperative laser-electron nuclear processes in atomic and molecular systems—New trend in quantum optics. European Physical Journal Special Topics. 2008;**160**(1):195–204

[93]   Glushkov AV, Malinovskaya SV. Co-operative laser nuclear processes: Border lines effects. In: Fazio G, Hanappe F, editors. New Projects and New Lines of Research in Nuclear Physics. Singapore: World Scientific; 2003. pp. 242–250

[94]   Glushkov AV, Khetselius OYu, Svinarenko AA, Prepelitsa GP. Energy approach to atoms in a laser field and quantum dynamics with laser pulses of different shape. In: Duarte FJ, editor. Coherence and Ultrashort Pulsed Emission. Rijeka: InTech; 2010. pp. 159–186