UDC 539.182

V. B. Ternovsky[1], M. Yu. Gurskaya[2], A. A. Svinarenko[2] , V. F. Mansarliysky[2]

[1]Odessa National Maritime Academy, Didrikhsona str. 4, Odessa, 65001
[2]Odessa State Environmental University, L'vovskaya str.15, Odessa, 65016
E-mail: ternovskyvb@gmail.com

THEORETICAL STUDYING SPECTRA OF YTTERBIUM ATOM ON THE BASIS OF RELATIVISTIC MANY-BODY PERTURBATION THEORY: RYDBERG RESONANCES

Theoretical studying the Rydberg autoionization resonances in spectra of the lanthanides atoms (ytterbium) is carried out within the relativistic many-body perturbation theory and generalized relativistic energy approach (Gell-Mann and Low S-matrix formalism). The zeroth approximation of the relativistic perturbation theory is provided by the optimized Dirac-Fock and Dirac-Kohn-Sham ones. 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. The accurate theoretical results on the autoionization $4f^{13}[^2F_{7/2}]6s^2np[5/2]_2$, $4f^{13} [^2F_{7/2}] 6s^2nf[5/2]_2$ resonances energies and widths are presented and compared with experimental data, obtained on the basis of the laser polarization spectroscopy method.

1. Introduction

This paper goes on our work on theoretical studying spectra and spectroscopic parameters for heavy atoms, namely, lanthanides atoms (see, for example [1-56]). Let us remind that an investigation of spectra, optical and spectral, radiative and autoionization characteristics for heavy elements atoms and multicharged ions is traditionally of a great interest for further development quantum atomic optics and atomic spectroscopy and different applications in plasma chemistry, astrophysics, laser physics etc. (see Refs. [1-10]).

Different atomic spectroscopy methods have been used in studying radiative and autoionization characteristics of atomic systems. The well known classical multi-configuration Hartree-Fock method allowed to get a great number of the useful spectral information about light and not heavy atomic systems. The multi-configuration Dirac-Fock method is the most reliable version of calculation for multielectron systems with a large nuclear charge. In these calculations the one- and two-particle relativistic and important exchange-correlation corrections are taken into account (see Refs. [1] and Refs. therein). However, one should remember about very complicated structure of spectra of the lanthanides atoms and necessity of correct accounting the different correlation effects such as polarization interaction of the valent quasiparticles and their mutual screening, iterations of a mass operator etc.).The known method of the model relativistic many-body perturbation theory has been earlier effectively applied to computing spectra of low-lying states for some lanthanides atoms too [2,3] (see also [2-6]). We use an analogous version of the perturbation theory (PT) to study the Rydberg states characteristics, however, the zeroth approximation is generated by the Dirac-Fock model. In Refs. [7-10] the similar version of the perturbation theory has been used with using the Dirac-Kohn-Sham zeroth approximation. This method is actively used in solving many tasks of quantum, atomic and nuclear physics [57-87]. Here we present the results of computing the Rydberg Yb $4f^{13} [^2F_{7/2}]$ $6s^2np[5/2]_2$, $4f^{13} [^2F_{7/2}] 6s^2nf[5/2]_2$ states energies and widths within both approaches and compare theoretical data with some experimental laser polarization spectroscopy method data [22,23]. All calculations are performed with using Superatom package (see for example, 2-24]).

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

As the method of computing is earlier presented in details, here we are limited only by the key topics. A model relativistic energy approach in a case of the multielectron atom has been proposed by Ivanov-Ivanova et al [2-4] and its generalized gauge-invariant version is developed in Refs. [5,6,11,2]. The approach is based on the Gell-Mann and Low S-matrix formalism and the relativistic many-body PT with using the optimized one-quasiparticle representation and an accurate account of the relativistic and exchange-correlation effects. In the relativistic case the Gell-Mann and Low formula expressed an energy shift ΔE through the QED scattering matrix including the interaction with as the photon vacuum field as the laser field . The wave function zeroth basis is found from the Dirac equation with a potential, which includes ab initio optimized model (Ivanov-Ivanova type [6]) potential or DF potentials, the electric potential of a nucleus (the Gaussian form of the charge distribution in a nucleus is usually used by us) [4]. The correlation corrections of the PT second and higher orders are taken into account by means of using the polarization and screening potentials (from Refs. [10-16]).

Generally speaking, 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 [2,11,12]. 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 ReΔE 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 [7-12] 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 [3,4,11]:

$$M = M^{(0)} + M^{(1)} + M^{(2)} + M^{(3)}, \qquad (1)$$

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 Re$M^{(2)}$ have been analyzed previously [4] using Feynman diagrams [11]. 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 [11-20]. 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 the Breit interaction has been taken as follows:

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

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 photo processes in the approximate calculations is a well known fact and is in details investigated by Grant, Armstrong, Aymar and Luc-Koenig, Glushkov-Ivanov et al (see [11] and numerous Refs. therein). 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 [1]. 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 [6]. Here we applied this approach for generating the optimized relativistic orbitals basis in the zeroth approximation of the many-body PT [7-10]. 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. Below we will be interested by studying the spectra of

the autoionization resonances in the ytterbium atom and calculating their energies and widths. The excited states of the ytterbium atom can be treated as the states with two-quasiparticles above the electron core [Xe]4f^{14}. Within the standard energy approach [8-11] the autoionization width is determined by the square of an electron interaction (3) matrix element. The real part of the electron interaction matrix element is determined using expansion in terms of Bessel functions [17-19,26]; the Coulomb part Q_λ^{Qul} is expressed in terms of the standard radial integrals and angular coefficients. The Breit part of Q is defined in the similar way as above, but the contribution of our interest is a real part. The Breit interaction is known to change considerably the autoionization decay dynamics in some cases (see, for example, Refs. [3,11]). Determination of the radiation decay probabilities (oscillator strengths) results to calculating the imaginary matrix elements of the interaction (3). The calculation of radial integrals ReR_λ(1243) is reduced to the solution of a system of differential equations according to the Ivanova-Ivanov method [26]. The system of differential equations includes also equations for functions $f/r^{|\ae|-1}$, $g/r^{|\ae|-1}$, $Z_\lambda^{(1)}$, $Z_\lambda^{(2)}$. The formulas for the autoionization decay probability include the radial integrals $R_\alpha(\alpha k \gamma \beta)$, where one of the functions describes electron in the continuum state. The correctly normalized function should have the following regular asymptotic at $r \to 0$ (look details in Refs. [13-19]). Other details can be found in Refs. [6-11,13-19].

3. Some illustration results and conclusion

In table 1 we present the experimental data (Jong-Hoon et al [87,88]) and theoretical results (Th1–PT with the Dirac-Kohn-Sham zeroth approximation [7,8]; Th2 – this work) for energies and widths of the excited (autoionization) states of the 4f^{13} [^{2}F$_{7/2}$]6s^{2}np[5/2]$_2$ and 4f^{13} [^{2}F$_{7/2}$] 6s^2 nf [5/2]$_2$ states (because of excitation of the 4f shell).

In table 2 we present the predictions of this work regarding the energies and widths of the excited (autoionization) states 4f^{13} [^{2}F$_{7/2}$] 6s^{2}nf [5/2]$_2$ states. As it has been noted in [5], the attention is drawn to the smallness of the resonance widths, the cause of which in the literature is not clear. In

our opinion, it is related to the complex energetic structure of the 4f-shell atoms, as a result of causing several unusual physics of autoionization resonances and their decay mechanisms, especially in comparison with the conventional standards spectroscopy (for He, inert gases, alkali atoms)

Table 1

Energies E (cm^{-1}), widths Γ (cm^{-1}) of the 4f^{13} [^{2}F$_{7/2}$]6s^{2}np[5/2]$_2$ states in YbI: Th1- PT with Dirac-Kohn-Sham zeroth approximation; Th2- Th1- PT with Dirac-Fock zeroth approximation (this work)

n	Exp. E_{exp}	Exp. Γ_{exp}	Th1. E	Th1. Γ	Th2. E	Th2. Γ
12	70120.5	1.5	70121	1.7	70123	1.6
15	70914.8	1.2	70916	1.4	70917	1.3
20	71428.1	0.6	71429	0.7	71430	0.6
25	71612.5	1.3	71611	1.5	71612	1.4
26	71633.3	0.6	71631	0.8	71633	0.7
30	71698.8	0.5	71697	0.7	71699	0.6
46	-	-	-	-	71798	0.3

It is important to note that the both perturbation theory versions with the Dirac-Fock and Dirac-Kohn-Sham zeroth approximations provide a physically reasonable agreement with experiment, however, more exact data are provided by the optimized Dirac-Fock-like theory.

Table 2

Energies E (cm^{-1}), widths Γ (cm^{-1}) of the 4f^{13} [^{2}F$_{7/2}$] 6s^2 nf [5/2]$_2$ states (predictions of this work)

n	Th. E	Th. Γ
12	70966	0.6
13	71109	0.4
15	71314	1.5
20	71562	0.8
25	71674	0.7
26	71690	0.6
30	71735	0.4
46	71814	0.2

References

1. Grant I.P., Relativistic Quantum Theory of Atoms and Molecules.-Oxford, 2008.-650P.
2. Ivanov L.N.,Ivanova E.P., Extrapolation of atomic ion energies by model potential method: Na-like spectra/ // Atom.Data Nucl .Data Tab.-1979.-Vol.24.-P.95-121.
3. Ivanov L.N., Letokhov V.S., Autoionization states of multielectron atoms// Com. Of Modern Phys. D. Atom. and Mol.Phys.-1985.-Vol.4.-P.169-184.
4. Ivanova E.P., Ivanov L.N., Glushkov A.V., Kramida A.E. High order corrections in the relativistic perturbation theory with the model zeroth approximation, My-like and Ne-like ions // Phys.Scripta −1985.-Vol.32,N4.-P.513.
5. Glushkov A.V., Ivanov L.N., Ivanova E.P., Radiation decay of atomic states. Generalized energy approach// Autoionization Phenomena in Atoms.- M.: Moscow State Univ.-1986. –P.58.
6. Glushkov A.V., Ivanov L.N. Radiation decay of atomic states: atomic residue polarization and gauge non-invariant contributions//Phys.Lett.A.-1992.-Vol. 170.-P.33-36.
7. Svinarenko A.A., Study of spectra for lanthanides atoms with relativistic many- body perturbation theory: Rydberg resonances// J. Phys.: Conf. Ser.-2014.-Vol.548.-P.012039.
8. Svinarenko A.A., Ignatenko A.V., Ternovsky V.B., Nikola V.V., Seredenko S.S., Tkach T.B., Advanced relativistic model potential approach to calculation of radiation transition parameters in spectra of multicharged ions// J. Phys.: Conf. Ser. -2014.-Vol.548.-P. 012047.
9. Svinarenko A.A., Khetselius O.Yu., Buyadzhi V.V., Florko T.A., Zaichko P.A., Ponomarenko E.L., Spectroscopy of Rydberg atoms in a Black-body radiation field: Relativistic theory of excitation and ionization// J. Phys.: Conf. Ser.-2014.-Vol.548.-P. 012048.
10. Svinarenko A.A., Nikola L. V., Prepelitsa G.P., Tkach T.B, Mischenko

E.V., Auger (autoionization) decay of excited states in spectra of multicharged ions: Relativistic theory//AIP Conf. Proceedings.-2010.-Vol.1290, N1 P.94-98.

11. Glushkov A.V., Relativistic and correlation effects in spectra of atomic systems.-Odessa: Astroprint.-2006.-400P.

12. Glushkov A.V., Atom in electromagnetic field.-Kiev: KNT, 2005.-450P.

13. Glushkov A.V., Khetselius O.Yu., Loboda A.V., Svinarenko A.A., QED approach to atoms in a laser field: Multiphoton resonances and above threshold ionization//Frontiers in Quantum Systems in Chemistry and Physics, Ser.: Progress in Theoretical Chemistry and Physics; Eds. S.Wilson, P.J.Grout, J. Maruani, G. Delgado-Barrio, P. Piecuch (Springer), 2008.-Vol.18.-P.543-560.

14. Glushkov A.V., Khetselius O.Y., Malinovskaya S.V., New laser-electron nuclear effects in the nuclear γ transition spectra in atomic and molecular systems// Frontiers in Quantum Systems in Chemistry and Physics. Series: Progress in Theoretical Chemistry and Physics Eds. S.Wilson, P.J.Grout, J. Maruani, G. Delgado-Barrio, P. Piecuch (Springer).-2008.-Vol.18.-525 p.

15. Glushkov A.V., Khetselius O.Yu., Svinarenko A.A., Prepelitsa G.P., Energy approach to atoms in a laser field and quantum dynamics with laser pulses of different shape//In: Coherence and Ultrashort Pulse Laser Emission, Ed. by Dr. F. Duarte (InTech).-2010.-P.159-186.

16. Glushkov A.V., Khetselius O. Yu., Svinarenko A. A., Relativistic theory of cooperative muon-γ gamma-nuclear processes: Negative muon capture and metastable nucleus discharge// Advances in the Theory of Quantum Systems in Chemistry and Physics. Ser.: Progress in Theor. Chem. and Phys., Eds. P.Hoggan, E.Brandas, J.Maruani, G. Delgado-Barrio, P.Piecuch (Springer).-2012.-Vol.22.-P.51.

17. Khetselius O.Yu., Relativistic calculating the hyperfine structure parameters for heavy-elements and laser detecting the isotopes and nuclear reaction products//Phys.Scripta.-2009.-T.135.-P.014023.

18. Glushkov A.V., Khetselius O.Yu., Lovett L., Electron-β-Nuclear Spectroscopy of Atoms and Molecules and Chemical Bond Effect on the β-Decay parameters// Advances in the Theory of Atomic and Molecular Systems Dynamics, Spectroscopy, Clusters, and Nanostructures. Series: Progress in Theor. Chem. and Phys., Eds. Piecuch P., Maruani J., Delgado-Barrio G., Wilson S. (Springer).-2009.-Vol.20.-P.125-152.

19. Glushkov A.V., Svinarenko A.A., Khetselius O.Yu., Buyadzhi V.V., Florko T.A., Shakhman A.N., Relativistic Quantum Chemistry: An Advanced approach to the construction of the Green function of the Dirac equation with complex energy and mean-field nuclear potential// Frontiers in Quantum Methods and Applications in Chem. and Physics. Ser.: Progress in Theor. Chem. and Phys., Eds. M. Nascimento, J.Maruani, E.Brändas, G. Delgado-Barrio (Springer).-2015-Vol.29.-P.197-217.

20. Malinovskaya S.V., Glushkov A.V., Dubrovskaya Yu.V., Vitavetskaya L.A., Quantum calculation of cooperative muon-nuclear processes: discharge of metastable nuclei during negative muon capture// Recent Advances in the Theory of Chemical and Physical Systems (Springer).-2006.-Vol.15.-P.301-307.

21. Malinovskaya S.V., Glushkov A.V., Khetselius O.Yu., Lopatkin Yu., Loboda A.V., Svinarenko A.A., Nikola L., Perelygina T., Generalized energy approach to calculating electron collision cross-sections for multicharged ions in a plasma: Debye shielding model// Int. Journ. Quant. Chem.-2011.-Vol.111.-P.288-296.

22. Malinovskaya S.V., Glushkov A.V., Khetselius O.Yu., Svinarenko A.A., Mischenko E.V., Florko T.A., Opti-

mized perturbation theory scheme for calculating the interatomic potentials and hyperfine lines shift for heavy atoms in the buffer inert gas//Int. Journ. Quant.Chem.-2009.-Vol.109,N14.-P.3325-3329.

23. Khetselius O.Yu., Optimized perturbation theory to calculating the hyperfine line shift and broadening for heavy atoms in the buffer gas// Frontiers in Quantum Methods and Applications in Chemistry and Physics. Ser.: Progress in Theor. Chem. and Phys., Eds. M.Nascimento, J.Maruani, E.Bröndas, G.Delgado-Barrio (Springer).-2015-Vol.29.-P.55-76.

24. Glushkov A.V., Ambrosov S.V., Loboda A.V., Gurnitskaya E.P., Khetselius O.Yu., QED calculation of heavy multi-charged ions with account for the correlation, radiative and nuclear effects// Recent Advances in Theor. Phys. and Chem. Systems.-2006.-Vol.15.-P.285.

25. Glushkov A.V.,Khetselius O.Yu., Gurnitskaya E.P., Korchevsky D.A., Loboda A.V., Prepelitsa G.P., Sensing the electron-collision excitation cross-sections for Ne-like ions of Fe in a plasma in the Debye shielding approximation// Sensor Electr. and Microsyst. Techn.-2007.-N2.-P.9-13

26. Glushkov A.V., Rusov V.D., Ambrosov S.V., Loboda A.,Resonance states of compound super-heavy nucleus and EPPP in heavy nucleus collisions//New projects and new lines of research in nuclear physics. Eds. G.Fazio, F.Hanappe, Singapore : World Scientific.-2003.-P.126-132.

27. Glushkov A.V., Malinovskaya S.V., Loboda A., Shpinareva I.M.,Gurnitskaya E., Korchevsky D., Diagnostics of the collisionally pumped plasma and search of the optimal plasma parameters of x-ray lasing: Calculation of electron-collision strengths and rate coefficients for Ne-like plasma// J. Phys.: Conf. Ser.-2005.-Vol.11.-P.188-198.

28. Glushkov A.V., Mansarliysky V.F., Khetselius O.Yu., Ignatenko A.V., Smirnov A., Prepelitsa G.P., Collisional shift of hyperfine line for thallium in an atmosphere of the buffer inert gas // Journal of Physics: C Series (IOP, London, UK).-2017.-Vol.810.-P. 012034.

29. Glushkov A.V., Malinovskaya S.V., Sukharev D.E., Khetselius O.Yu., Loboda A.V., Lovett L., Green's function method in quantum chemistry: New numerical algorithm for the Dirac equation with complex energy and Fermi-model nuclear potential//Int.Journ. Quant.Chem.-2009.-Vol. 109.-N8.-P.1717-1727.

30. Glushkov A.V., Khetselius O.Yu., Gurnitskaya E.P., Florko T.A., Sensing of nuclei available in little quantities by means of laser spectroscopy of hyperfine structure for isotopes: new theoretical scheme (U ,Hg) // Sensor Electr. and Microsyst. Techn.-2007.-N3.-P.8-12

31. Glushkov A.V., Kondratenko P.A., Lepikh Ya., Fedchuk A.P., Svinarenko A.A., Lovett L., Electrodynamical and quantum - chemical approaches to modelling the electrochemical and catalytic processes on metals, metal alloys and semiconductors//Int. Journ. Quantum Chem..-2009.-Vol.109,N14.-P.3473-3481.

32. Glushkov A.V., Malinovskaya S.V., New approach to the formation of model potential for valence-electrons// Zhurn.Fizich.Khimii.-1988.-Vol.62(1).-P.100-104.

33. Ternovsky V.B., Glushkov A.V., Zaichko P.A., Khetselius O.Yu., Florko T.A., New relativistic model potential approach to sensing radiative transitions probabilities in spectra of heavy Rydberg atomic systems/ // Sensor Electr. and Microsyst. Techn.-2015.-Vol.12,N4.-P.19-26.

34. Buyadzhi V.V., Glushkov A.V., Mansarliysky V.F., Ignatenko A.V., Svinarenko A.A., Spectroscopy of atoms in a strong laser field: New method to sensing AC Stark effect, multiphoton resonances parameters and ionization cross-sections//Sensor Electr. and Microsyst. Techn.-2015.-Vol.12,N4.-P.27-36.

35. Glushkov A.V., Effective quasi-particle valence hamiltonian of molecules in the comprehensive semi-empirical theory// Sov. Journ. Struct. Chem.-1988.-Vol.29,N4.-P.3-9.

36. Glushkov A.V., Khetselius O.Yu., Lopatkin Y., Florko T.A., Kovalenko O., Mansarliysky V.F., Collisional shift of hyperfine line for rubidium in an atmosphere of the buffer inert gas//J. Phys.:Conf.Series.-2014.-Vol.548.-P.012026

37. Glushkov A.V., Khetselius O.Yu., Bunuakova Yu.Ya., Buyadzhi V.V, Brusentseva S.V., Zaichko P.A., Sensing interaction dynamics of chaotic systems within a chaos theory and microsystem technology Geomath with application to neurophysiological systems// Sensor Electr. and Microsyst.Techn.-2014.-Vol. 11,N3.-P.62-69.

38. Prepelitsa G.P., Glushkov A.V., Lepikh Ya.I., Buyadzhi V.V., Ternovsky V.B., Zaichko P.A., Chaotic dynamics of nonlinear processes in atomic and molecular systems in electromagnetic field and semiconductor and fiber laser devices: new approaches, uniformity and charm of chaos// Sensor Electr. and Microsyst. Techn.-2014.-Vol.11,N4.-P.43-57.

39. Khetselius O.Yu., Hyperfine structure of atomic spectra.-Odessa: Astroprint, 2008.-210P.

40. Khetselius O.Yu., Hyperfine structure of radium// Photoelectronics.-2005.-N14.-P.83-85.

41. Khetselius O.Yu., Spectroscopy of co-operative electron-gamma-nuclear processes in heavy atoms: NEET effect// J. Phys.: Conf. Ser.-2012.- Vol.397.-P.012012

42. Khetselius O.Yu., Florko T.A., Svinarenko A.A., Tkach T.B., Radiative and collisional spectroscopy of hyperfine lines of the Li-like heavy ions and Tl atom in an atmosphere of inert gas//Phys.Scripta.-2013.-Vol.T153-P.014037.

43. Khetselius O.Yu., Turin A.V., Sukharev D.E., Florko T.A., Estimating of X-ray spectra for kaonic atoms as tool for sensing the nuclear structure// Sensor Electr. and Microsyst. Techn.-2009.-N1.-P.30-35.

44. Khetselius O.Yu., On possibility of sensing nuclei of the rare isotopes by means of laser spectroscopy of hyperfine structure//Sensor Electr. and Microsyst.Techn.-2008.-Vol.3.-P.28-33.

45. Khetselius O.Yu., Quantum Geometry: New approach to quantization of the quasistationary states of Dirac equation for super heavy ion and calculating hyperfine structure parameters// Proc. Int. Geometry Center.-2012.-Vol.5,№ 3-4.-P.39-45.

46. Glushkov A.V., Khetselius O.Yu., Svinarenko A.A., Theoretical spectroscopy of autoionization resonances in spectra of lanthanide atoms// Physica Scripta.-2013.-Vol.T153.-P.014029.

47. Glushkov A.V., Khetselius O.Yu., Gurnitskaya E.P., Loboda A.V., Sukharev D.E., Relativistic quantum chemistry of heavy ions and hadronic atomic systems: spectra and energy shifts// Theory and Applications of Computational Chemistry. AIP Conference Proceedings.-2009.-Vol.1102.-P.168-171.

48. Khetselius O.Yu., Relativistic calculating the spectral lines hyperfine structure parameters for heavy ions//Spectral Line Shapes, AIP Conf. Proceedings.-2008.-Vol.1058.-P.363-365.

49. Khetselius O.Yu., Glushkov A.V., Gurnitskaya E.P., Loboda A.V., Mischenko E.V., Florko T.A., Sukharev D.E., Collisional Shift of the Tl hyperfine lines in atmosphere of inert gases// Spectral Line Shapes, AIP Conf. Proceedings.-2008.-Vol.1058.-P.231-233.

50. Khetselius O.Yu., Hyperfine structure of energy levels for isotopes 73Ge, 75As, 201Hg// Photoelectronics.-2007.-N16.-P.129-132.

51. Khetselius O.Y., Gurnitskaya E.P., Sensing the electric and magnetic moments of a nucleus in the N-like ion of Bi// Sensor Electr. and Microsyst.

Techn.-2006.-N3.-P.35-39.

52. Khetselius O.Y., Gurnitskaya E.P., Sensing the hyperfine structure and nuclear quadrupole moment for radium// Sensor Electr. and Microsyst. Techn.-2006.-N2.-P.25-29.

53. Florko T.A., Loboda A.V., Svinarenko A.A., Sensing forbidden transitions in spectra of some heavy atoms and multicharged ions: New theoretical scheme// Sensor Electr. and Microsyst. Techn.-2009.-N3.-P.10-15.

54. Sukharev D.E., Khetselius O.Yu., Dubrovskaya Yu.V., Sensing strong interaction effects in spectroscopy of hadronic atoms// Sensor Electr. and Microsyst. Techn.-2009.-N3.-P.16-21.

55. Glushkov A.V., Khetselius O.Yu., Loboda A.V., Ignatenko A., Svinarenko A., Korchevsky D., Lovett L., QED approach to modeling spectra of the multicharged ions in a plasma: Oscillator and electron-ion collision strengths// Spectral Line Shapes. AIP Conference Proceedings.-2008.-Vol.1058.-P.175-177

56. Glushkov A.V., Ambrosov S.V., Loboda A., Gurnitskaya E.P., Prepelitsa G.P., Consistent QED approach to calculation of electron-collision excitation cross-sections and strengths: Ne-like ions//Int. Journ.Quant.Chem.-2005.-Vol.104, N4 .-P. 562-569.

57. Glushkov A.V.,Lepikh Ya.I.,Khetselius O.Yu., Fedchuk A.P., Ambrosov S.V , Ignatenko A.V., Wannier-mott excitons and atoms in a DC elecric field: photoionization, Stark effect, resonances in the ionization continuum// Sensor Electr. and Microsyst. Techn.-2008.-N4.-P.5-11.

58. Khetselius O.Yu., Relativistic energy approach to cooperative electron-γ-nuclear processes: NEET Effect// Quantum Systems in Chemistry and Physics: Progress in Methods and Applications. Ser.: Progress in Theor. Chem. and Phys., Eds. K.Nishikawa, J. Maruani, E.Brandas, G. Delgado-Barrio, P.Piecuch (Springer).-

2012-Vol.26.-P. 217.

59. Buyadzhi V.V., Glushkov A.V., Lovett L., Spectroscopy of atoms and nuclei in a strong laser field: AC Stark effect and multiphoton resonances// Photoelectronics.-2014.-Vol.23.-P. 38-43.

60. Glushkov A.V., Ambrosov S.V., Ignatenko A.V., Korchevsky D.A., DC Strong Field Stark effect for non-hydrogenic atoms: Consistent quantum mechanical approach// Int.Journ. Quant. Chem.-2004.-Vol.99,N6.-P.936-939.

61. Glushkov A.V, Malinovskaya S.V, Chernyakova Y.G., Svinarenko A.A., Cooperative laser-electron-nuclear processes: QED calculation of electron satellites spectra for multi-charged ion in laser field// Int. Journ. Quant. Chem.-2004.-Vol.99,N6.-P.889-893.

62. Glushkov A.V, Khetselius O.Yu, Malinovskaya S.V, Optics and spectroscopy of cooperative laser-electron nuclear processes in atomic and molecular systems - new trend in quantum optics// Europ. Phys. Journ. ST.-2008.-Vol.160,N1.-P.195-204.

63. Glushkov A.V., Malinovskaya S.V, Gurnitskaya E.P., Khetselius O.Yu.,Dubrovskaya Yu.V., Consistent quantum theory of the recoil induced excitation and ionization in atoms during capture of neutron// Journal of Physics: Conf. Series (IOP).-2006.- Vol.35.-P.425-430.

64. Glushkov A.V., Dan'kov S.V., Prepelitsa G., Polischuk V.N., Efimov A., Qed theory of nonlinear interaction of the complex atomic systems with laser field multi-photon resonances// Journal of Tech. Phys.-1997.-Vol.38 (2).-P.219-222

65. Glushkov A.V., Calculation of parameters of the interaction potential between excited alkali atoms and mercury atoms - the Cs-, Fr-Hg interaction// Optika i Spektr.-1994.-Vol.77 (1).-P.5-10.

66. Glushkov A.V., Khetselius O.Yu., Prepelitsa G.P., Svinarenko A.A., Geometry of Chaos I: Theoretical basis's of

a consistent combined approach//Proc. Int. Geometry Center.-2013.-Vol.6, N1.-P.67-79.

67. Chernyakova Yu.G., Dubrovskaya Yu.V., Florko T.A., Romanova A.V., Vitavetskaya L., An advanced approach to quantization of the quasi stationary states of Dirac-Slater equation// Proc. Int. Geometry Center.-2013.-Vol.6,N2.-P.29-34.

68. Glushkov A.V., Khetselius O., Dubrovskaya Yu.V., Loboda A.V., Sensing the capture of negative muon by atoms: Energy approach// Sensor Electr. and Microsyst. Techn.-2006.-N4.-P.31-35.

69. Glushkov A.V., Svinarenko A.A., Nuclear quantum optics: Energy approach to multi-photon resonances in nuclei // Sensor Electr. and Microsyst. Techn.-2010.-N2.-P.5-10.

70. Glushkov A.V., Energy approach to resonance states of compound super-heavy nucleus and EPPP in heavy nuclei collisions// Low Energy Antiproton Phys. AIP Conference Proceedings.-2005.-Vol.796.-P.206-210.

71. Malinovskaya S.V., S.V., Dubrovskaya Yu., Vitavetskaya L., Advanced quantum mechanical calculation of the beta decay probabilities// Low Energy Antiproton Phys. AIP Conference Proceedings.-2005.-Vol.796.-P.201-205.

72. Glushkov A.V., Khetselius O.Yu., Svinarenko A.A., Lovett L., Energy approach to nuclei and atoms in a strong laser field: Stark effect and multi-photon resonances // Quantum Theory: Reconsideration of Foundations. AIP Conference Proceedings.-2010.-Vol.1232.-P.228-234.

73. Glushkov A.V., Lovett L., Khetselius O.Yu., Gurnitskaya E.P., Dubrovskaya Yu.V., Loboda A.V., Generalized multiconfiguration model of decay of multipole giant resonances applied to analysis of reaction (μ-n) on the nucleus ^{40}Ca// Internat. Journ. Modern Physics A.-2009.- Vol. 24, N.2-3.-P.611-615.

74. Svinarenko A.A., Glushkov A.V., Loboda A.V., Sukharev D.E., Dubrovskaya Yu.V., Mudraya N.V., Serga I.N., Green's function of the Dirac equation with complex energy and non-singular central nuclear potential//Quantum Theory: Reconsideration of Foundations. AIP Conf. Proceedings.-2010.-Vol.1232.-P.259-266.

75. Glushkov A.V., Loboda A.V., Gurnitskaya E., Svinarenko A.A., QED theory of radiation emission and absorption lines for atoms in a strong laser field// Phys. Scripta.-2009.-T.135.-P. 014022.

76. Glushkov A.V., Malinovskaya S.V., Prepelitsa G.P., Ignatenko V.M., Manifestation of the new laser-electron nuclear spectral effects in thermalized plasma: QED theory of cooperative laser-electron- nuclear processes//J. Phys.:Conf. Ser.-2005.-Vol.11.-P.199-206.

77. Glushkov A.V., Malinovskaya S.V., Ambrosov S., Shpinareva I.M., Troitskaya O.V., Resonances in quantum systems in strong external fields consistent quantum approach// J. of Techn.Phys.-1997.-Vol.38, Iss.2.-P.215-218.

78. Buyadzhi V.V., Zaichko P.A., Gurskaya M., Kuznetsova A.A., Ponomarenko E.L., Ternovsky V.B., Relativistic theory of excitation and ionization of Rydberg atoms in a Black-body radiation field//J. Phys.: Conf. Series.-2017.-Vol.810.-P. 012047.

79. Glushkov A.V., Spectroscopy of atom and nucleus in a strong laser field: Stark effect and multiphoton Resonances// J.Phys.: Conf. Series (IOP).-2014.-Vol.548.-P.012020.

80. Glushkov A.V., Kondratenko P.A., Buyadzhi V.V., Kvasikova A.S., Shakhman A.S., Sakun T.N., Spectroscopy of cooperative laser electron-γ-nuclear processes in polyatomic molecules// J. Phys.: Conf. Ser.-2014.-Vol.548.-P.012025

81. Glushkov A.V., Khetselius O.Yu., Prepelitsa G.P., Svinarenko A.A., Geometry of Chaos: Theoretical basis's of a consistent combined approach to treating chaotic dynamical systems and their parameters determination //Proc. of In-

ternational Geometry Center".-2013.-Vol.6, N1.-P.43-48.

82. Glushkov A.V., Khetselius O.Yu., Malinovskaya S.V., Spectroscopy of co-operative laser-electron nuclear effects in multiatomic molecules// Molec. Phys. (UK).-2008.-Vol.106.-N9-10.-P.1257-1260.

83. Glushkov A.V., Khetselius O.Yu., Svinarenko A.A., Prepelitsa G.P., Mischenko E.V., The Green's functions and density functional approach to vibrational structure in the photoelectron spectra for molecules// AIP Conf. Proceedings.-2010.-Vol.1290.-P. 263-268.

84. Glushkov A.V, Malinovskaya S.,Co-operative laser nuclear processes: border lines effects// In: New projects and new lines of research in nuclear physics. Eds. G.Fazio and F.Hanappe, Singapore : World Scientific.-2003.-P.242-250.

85. Khetselius O. Yu., Florko T. A., Nikola L., Svinarenko A., Serga I., Tkach T., Mischenko E., Hyperfine structure, scalar-pseudoscalar interaction and parity non-conservation effect in some heavy atoms and ions// Quantum Theory: Reconsideration of Foundations. AIP Conference Proceedings.-2010.-Vol.1232.-P.243-250.

86. Glushkov A.V., Operator Perturbation Theory for Atomic Systems in a Strong DC Electric Field//Advances in Quantum Methods and Applications in Chemistry, Physics, and Biology. Series: Frontiers in Theoretical Physics and Chemistry, Eds. M.Hotokka, J.Maruani, E. Brändas, G.Delgado-Barrio (Springer).-2013.-Vol. 27.-P.161-177.

87. Jong-hoon Yi, Lee J., Kong H.J., Auto-ioni-zing states of the ytterbium atom by three-photon polarization spectroscopy//Phys. Rev. A.-1995.-Vol.51.-P.3053–3057.

88. Jong-hoon Yi, Park H., Lee J., Investigation of even parity autoionizing states of ytterbium atom by two-photon ionization spectroscopy//J. Kor.Phys.Soc.-2001.-Vol.39. -P.916-920.

V. B. Ternovsky, M. Yu. Gurskaya, A. A. Svinarenko, V. F. Mansarliysky

THEORETICAL STUDYING SPECTRA OF YTTERBIUM ATOM ON THE BASIS OF RELATIVISTIC MANY-BODY PERTURBATION THEORY: RYDBERG RESONANCES

Summary

Theoretical studying the Rydberg autoionization resonances in spectra of the lanthanides atoms (ytterbium) is carried out within the relativistic many-body perturbation theory and generalized relativistic energy approach (Gell-Mann and Low S-matrix formalism). The zeroth approximation of the relativistic perturbation theory is provided by the optimized Dirac-Fock and Dirac-Kohn-Sham ones. 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. The accurate theoretical results on the autoionization $4f^{13}[^2F_{7/2}]6s^2np[5/2]_2$, $4f^{13}[^2F_{7/2}]6s^2nf[5/2]_2$ resonances energies and widths are presented and compared with experimental data, obtained on the basis of the laser polarization spectroscopy method.

Keywords: Relativistic perturbation theory, resonances energies and widths, optimized zeroth approximation

УДК 539.182

В. Б. Терновский, М. Ю. Гурская, А. А. Свинаренко, В. Ф. Мансарлийский

ТЕОРЕТНЧЕСКОЕ НЗУЧЕННЕ СПЕКТРА АТОМА НТЕРБИЯ НА ОСНОВЕ РЕЛЯТНВНСТСКОЙ МНОГОЧАСТНЧНОЙ ТЕОРНН ВОЗМУЩЕННЙ: РИДБЕРГОВЫ РЕЗОНАНСБ

Резюме

В рамках релятивистской многочастичной теории возмущений и обобщенного релятивистского энергетического подхода проведено теоретическое изучение характеристик ридберговских автоионизационных резонансов в спектрах атомов лантанидов (иттербия). В качестве нулевого приближения релятивистской теории возмущений выбраны оптимизированные приближения Дирака-Фока и Дирака-Кона-Шэма. Оптимизация выполнена путем введения параметра в обменные потенциалы Фока и Кона-Шэма и дальнейшей минимизацией калибровочно-неинвариантных вкладов в радиационные ширины атомных уровней с использованием релятивистских орбитальных базисов, сгенерированных соответствующими гамильтонианами нулевого приближения. Представлены аккуратные теоретические данные по энергиям и ширинам автоионизационных $4f^{13}[^2F_{7/2}]6s^2np[5/2]_2$, $4f^{13}$ $[^2F_{7/2}]$ $6s^2nf[5/2]_2$ резонансов и проведено сравнение с экспериментальными данными, полученными на основе метода лазерной поляризационной спектроскопии.

Ключевые слова: Релятивистская теория возмущений, энергии и ширины резонансов, оптимизированное нулевое приближение

УДК 539.182

В. Б. Терновський, М. Ю. Гурська, А. А. Свинаренко, В. Ф. Мансарлійський

ТЕОРЕТИЧИЕ ВИВЧЕННЯ СПЕКТРА АТОМА ІТЕРБІЮ НА ОСНОВІ РЕЛЯТНВІСТСБКОЇ БАГАТОЧАСТННКОВОЇ ТЕОРІЇ ЗБУРЕНБ: РІДБЕРГОВІ РЕЗОНАНСН

Резюме

В рамках релятивістської багаточастинкової теорії збурень і узагальненого релятивістського енергетичного підходу проведено теоретичне вивчення характеристик рідбергівських автоіонізаційних резонансів в спектрах атомів лантанідів (ітербію). В якості нульового наближення релятивістської теорії збурень обрані оптимізовані наближення Дірака-Фока і Дірака-Кона-Шема. Оптимізація виконана шляхом введення параметра в обмінні потенціали Фока і Кона-Шема і подальшої мінімізації калібрувально-неінваріантних вкладів в радіаційні ширини атомних рівнів з використанням релятивістських орбітальних базисів, згенерованими відповідними гамільтоніанами нульового наближення, Представлені акуратні теоретичні дані по енергіях і ширинам автоіонізаційних $4f^{13}[^2F_{7/2}]6s^2np[5/2]_2$, $4f^{13}$ $[^2F_{7/2}]$ $6s^2nf[5/2]$ резонансів і проведено порівняння з експериментальними даними, отриманими на основі методу лазерної поляризаційної спектроскопії.

Ключові слова: Релятивістська теорія збурень, енергії і ширини резонансів, оптимізоване нульове наближення