MINISTRY OF EDUCATION AND SCIENCE UKRAINE

ODESSA I. I. MECHNIKOV NATIONAL UNIVERSITY

ФОТОЭЛЕКТРОНИКА

PHOTOELECTRONICS
INTER-UNIVERSITIES SCIENTIFIC ARTICLES

Founded in 1986

Number 26

ODESSA
ONU
2017

«PHOTOELECTRONICS»
№ 26–2017

INTER-UNIVERSITIES SCIENTIFIC ARTICLES

Founded in 1986

Certificate of State Registration KB No 15953

«ФОТОЭЛЕКТРОНИКА»
№ 26–2017

МЕЖВЕДОМСТВЕННЫЙ НАУЧНЫЙ СБОРНИК

Основан в 1986 г.

Свидетельство о Государственной регистрации КВ № 15953

UDC 621.315.592:621.383.51:537.221

The results of theoretical and experimental studies in problems of the semiconductor and microelectronic devices physics, opto- and qantum electronics, quantum optics, spectroscopy and photophysics of nucleus, atoms, molecules and solids are presented in the issue. New directions in the photoelectronics, stimulated by problems of the super intense laser radiation interaction with nuclei, atomic systems and substance, are considered. Scientific articles «Photoelectronics» collection abstracted in ВИНИТИ and «Джерело»

Scientific articles «Photoelectronics» collection abstracted in ВИНИТИ and «ДЖЕРЕЛО»,and are in scientific-metric base INDEX COPERNICUS.

For lecturers, scientists, post-graduates and students.

У збірнику наведено результати теоретичних і експериментальних досліджень з питань фізики напівпровідників та мікроелектронних приладів, опто- та квантової електроніки, квантової оптики, спектроскопії та фотофізики ядра, атомів, молекул та твердих тіл. Розглянуто нові напрямки розвитку фотоелектроніки, пов'язані із задачами взаємодії надінтенсивного лазерного випромінювання з ядром, атомними системами, речовиною.

Збірник «Photoelectronics» реферується у ВІНІТІ (Москва) та «Джерело» (Київ) і знаходиться у науковометричній базі INDEX COPERNICUS

Для викладачів, наукових працівників, аспіранів, студентів

В сборнике приведены результаты теоретических и экспериментальных исследований по вопросам физики полупроводников и микроэлектронных приборов, опто- и квантовой электроники, квантовой оптики, спектроскопии и фотофизики ядра, атомов, молекул и твердых тел. Рассмотрены новые направления развития фотоэлектроники, связанные с задачами взаимодействия сверхинтенсивного лазерного излучения с ядром, атомными системами, веществом.

Сборник «Photoelectronics» реферируется в ВИНИТИ (Москва) и «Джерело» (Киев) и находится в наукометричной базе INDEX COPERNICUS

Для преподавателей, научных работников, аспирантов, студентов

Address of editorial board:

Odessa I. I. Mechnikov National University 42, Pasteur str., Odessa, 65026, Ukraine
Information is on the site: http://phys.onu.edu.ua/journals/photoele/
http://experiment.onu.edu.ua/exp_ru/files/?
e – mail:photoelectronics@onu.edu.ua.

TABLE OF CONTENT:

A. P. Chebanenko, L. M. Filevska, V. A. Smyntyna, N. S. Simanovich, V. S. Grinevych
THE HUMIDITY AND STRUCTURING ADDITIVES INFLUENCE
ON ELECTROPHYSICAL CHARACTERISTICS OF TIN DIOXIDE FILMS 5

A. V. Glushkov, V. B. Ternovsky, A. A. Svinarenko, A. V. Smirnov
GAUGE-INVARIANT RELATIVISTIC PERTURBATION THEORY
APPROACH TO DETERMINATION OF ENERGY and SPECTRAL
CHARACTERISTICS FOR HEAVY AND SUPERHEAVY ATOMS
AND IONS: REVIEW 11

O. Yu. Khetselius, A. V. Glushkov, V. V. Buyadzhi, Yu. Ya. Bunyakova
NEW NONLINEAR CHAOS-DYNAMICAL ANALYSIS OF ATMOSPHERIC
RADON ^{222}Rn CONCENTRATION TIME SERIES FROM BETA PARTICLES
ACTIVITY DATA OF RADON MONITORS 29

Yu. A. Nitsuk, Yu. F. Vaksman, I. V. Tepliakova, A. A. Rimashevskiy
SYNTHESIS AND LUMINESCENCE PROPERTIES OF ZnSe:Al NANOPARTICLES 41

V. F. Mansarliysky, E. V. Ternovsky, A. V. Ignatenko, E. L. Ponomarenko
OPTIMIZED RELATIVISTIC DIRAC-FOCK APPROACH TO CALCULATING
THE HYPERFINE LINE SHIFT AND BROADENING FOR HEAVY ATOMS
IN THE BUFFER GAS 46

Yu. V. Dubrovskaya, A. A. Kuznetsova, A. S. Kvasikova, T. N. Sakun
SPECTROSCOPY OF COOPERATIVE ELECTRON-γ-NUCLEAR EFFECTS
IN MULTIATOMIC MOLECULES: MOLECULE XY_4 55

Ie. V. Brytavskyi, A. V. Tereshchenko, V. B. Myndrul, M. M. Pavlenko, V. A. Smyntyna
SILICON NANOPILLARS FORMING AND COVERING BY Zn AND Ti OXIDES
FOR SOLAR ENERGY APPLICATIONS AND BIOSENSORICS 62

I. N. Serga, O. Yu. Khetselius, L. A. Vitavetskaya, A. N. Bystryantseva
RELATIVISTIC THEORY OF SPECTRA OF THE PIONIC ATOMIC
SYSTEM ^{208}Pb WITH ACCOUNT OF STRONG PION-NUCLEAR INTERACTION
EFFECTS: 68

A. A. Kuznetsova, Yu. V. Dubrovskaya, A. V Glushkov, Ya. I. Lepikh
ADVANCED GREEN'S FUNCTIONS AND DENSITY FUNCTIONAL APPROACH
TO VIBRATIONAL STRUCTURE IN THE PHOTOELECTRON SPECTRA
OF DIATOMIC MOLECULE 78

A. O. Karpenko
A METHOD FOR LOWERING THE LEVEL OF THE ELECTROMAGNETIC WAVES
BACKGROUND RADIATION OF HORN RADIATOR 88

V. V. Buyadzhi, Yu. G. Chernyakova, O. A. Antoshkina, T. B. Tkach
SPECTROSCOPY OF MULTICHARGED IONS IN PLASMAS:
OSCILLATOR STRENGTHS OF Be-LIKE ION Fe 94

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 103

A. V. Smirnov, O. Yu. Khetselius, V. V. Buyadzhi, A. S. Belodonov
ADVANCED RELATIVISTIC APPROACH IN SPECTROSCOPY OF COMPLEX
AUTOIONIZATION RESONANCES IN ATOMIC SPECTRA.....114

N. S. Simanovych, Ye. V. Brytavskyi, M. I. Kutalova, V. A. Borshchak, Y. N. Karakis
THE STUDY OF HETEROGENEOUS SENSITIZED CRYSTALS OF CADMIUM
SULFIDE. PART I ABOUT CHARGE OF THE CENTERS RECOMBINATION..... 124

E. V. Ternovsky, O. A. Antoshkina, T. A. Florko, T. B. Tkach
RELATIVISTIC CALCULATION OF OSCILLATOR STRENGTHS OF THE
RADIATION TRANSITIONS BETWEEN BARIUM RYDBERG STATES..... 139

M. Yu. Gurskaya, A. V. Ignatenko, A. S. Kvasikova, A. A. Buyadzhi
ADVANCED DATA FOR HYDROGEN ATOM IN CROSSED ELECTRIC
AND MAGNETIC FIELDS 148

O. O. Ptashchenko, F. O. Ptashchenko, V. R. Gilmutdinova
EFFECT OF WATER VAPORS ON THE TIME-RESOLVED SURFACE
CURRENT INDUCED BY AMMONIA MOLECULES ADSORPTION
IN GaAs *P-N* JUNCTIONS 156

ІНФОРМАЦІЯ ДЛЯ АВТОРІВ НАУКОВОГО ЗБІРНИКА
«PHOTOELECTRONICS» 158

ИНФОРМАЦИЯ ДЛЯ АВТОРОВ НАУЧНОГО СБОРНИКА «PHOTOELECTRONICS» 159

INFORMATION FOR CONTRIBUTORS OF “PHOTOELECTRONICS” ARTICLES 160

PACS 73.61.Le, 73.63.Bd

A. P. Chebanenko, L. M. Filevska, V. A. Smyntyna, N. S. Simanovich, V. S. Grinevych

Odessa I. I. Mechnikov National University, Dvoryanskaya str.,2, Odessa, 65082, Ukraine,
e-mail: *lfilevska@gmail.com*

THE HUMIDITY AND STRUCTURING ADDITIVES INFLUENCE ON ELECTROPHYSICAL CHARACTERISTICS OF TIN DIOXIDE FILMS

The structuring additive concentration and humidity influence on the electrophysical properties of tin dioxide films was studied. The growth of SnO_2 films, interelectrode resistance with the growth of polyvinyl acetate concentration in the initial solution is due to the porosity increase caused by the PVA increase in the films under study. The section of dark current temperature dependence, in vacuum from 110 °C with an activation energy ~ 0.7 eV, is due to the water molecules desorption. The resistance decrease of tin dioxide films in a wet atmosphere due to the dissociative adsorption of water molecules on the SnO_2 layers surfaces has been established.

1. Introduction

Tin dioxide, an n-type semiconductor with a band gap of about 3.6 eV (at 300 K), belongs to the group of "transparent conductive oxides" (PPO), together with compounds such as ZnO, In_2O_3, WO_3, etc. Thin films of this oxide are transparent in the visible and near-UV spectrum region and at the same time may have high electrical conductivity, which makes them enough promising and even necessary material for transparent electrodes of solar cells, flat monitors, LEDs. [1-3].

Nanostructuring of thin SnO_2 films increases their porosity and, consequently, the effective area of their surface. Due to this, the conductivity of such films is particularly strongly affected by sorption processes occurring on their surface. As a result, many of the electrophysical properties of tin dioxide thin films prove to be highly sensitive to the film's interaction with various media, including gaseous and liquid media [4].

Many biological media, including various gases (CO, CO_2, SO_2, H_2S, nitrogen oxides, oxygen, ozone, etc.), as well as liquids (with the presence of different ions) interacting with tin dioxide films surfaces also can cause changes in their electrical characteristics. This property of tin dioxide makes it to be one of the most popular materials for the environment monitoring and various biological environments diagnostics. The influence of atmospheric air humidity on the tin dioxide conductivity should always be taken into account when using this material, both as a sensor and an electrode.

This work is intended to study the influence of both the humidity and of the structural additive amount in a fabrication solution on the electrophysical characteristics of tin dioxide films.

2. The film's fabrication methods and experiment

Thin films of nanostructured tin dioxide were obtained using polymer materials by the sol-gel method [5]. Bis-(acetylacetonato)dichlorotin (BADCT) was used as the tin precursor of tin dioxide [6]. Polyvinyl acetate (PVA) was used as a structuring polymer material. After coating the glass substrate by the initial solution, the samples were annealed to remove organic constituents and form a tin dioxide layer.

The registration of the electrophysical characteristics of SnO_2 nanofilms is based on the standard fixation of the I-U characteristics (CVC) and the Dark Current Temperature Dependence (DCTD). Indium was used as the electrode material. It was thermally deposited on the surface of the films in a high vacuum in the form of two parallel strips. The distance between the electrodes was 2 mm.

3. Results and discussion

Figure 1 shows the current-voltage characteristics for two films with the same precursor content (10%) and different PVA content, measured at room temperature in air. It can be noted that they are practically linear and only in the region of high voltages (more than 200 V) there is a tendency to a superlinear exponential current–voltage dependence.

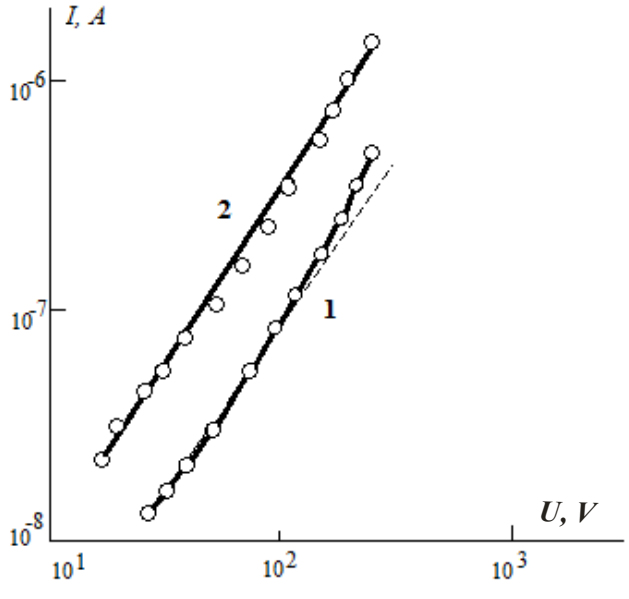


Fig. 1. The current-voltage characteristics of SnO_2 samples with a precursor content of 10% and PVA of 1% - curve 1, PVA 0.1% - curve 2 measured in air (T = 293 K).

Such behavior of the CVC was described in [7] and is associated with a change in the barrier height at the grain boundaries and electron tunneling through surface states.

From the comparison of curves 1 and 2 (Fig.1), it is seen that the interelectrode resistance of the films increases with PVA concentration growth (calculated from curve 1, $R = 1.2 \cdot 10^9$ Ω, calculated from curve 2, $R = 4.3 \cdot 10^8$ Ω). This becomes understandable, if it is taken into acount that polyvinyl acetate used in the preparation of films by the sol-gel method, plays the role of an organic filler and decomposes during high-temperature annealing, and the products of its decomposition volatilize. This causes the porosity and the development of the resulting films surfaces, which are more manifested, the larger the concentration of PVA in the initial solution.

Curve 1, Fig. 2 shows the current-voltage characteristic of SnO_2 film, measured at room temperature in air. The interelectrode resistance calculated from this CVC is $1.4 \cdot 10^9$ Ohm. Curve 2 depicts the current-voltage characteristic of the same SnO_2 film measured in a vacuum after the film was heated to a temperature of +150 °C and then cooled to room temperature in vacuum.

The interelectrode resistance calculated from it was $1.3 \cdot 10^8$ Ohm. Thus, heat treatment in vacuum causes the resistances reduce of SnO_2 film by almost an order of magnitude. This is due to the fact that under normal conditions, the oxygen adsorbed on the surface of SnO_2 film, captures electrons from the SnO_2 conduction band which results in the formation of positive space charge layer in the near surface region and, as a consequence, the energy bands curvature is of the cut off type. Since the films under investigation are thin, this causes a noticeable increase in their resistance.

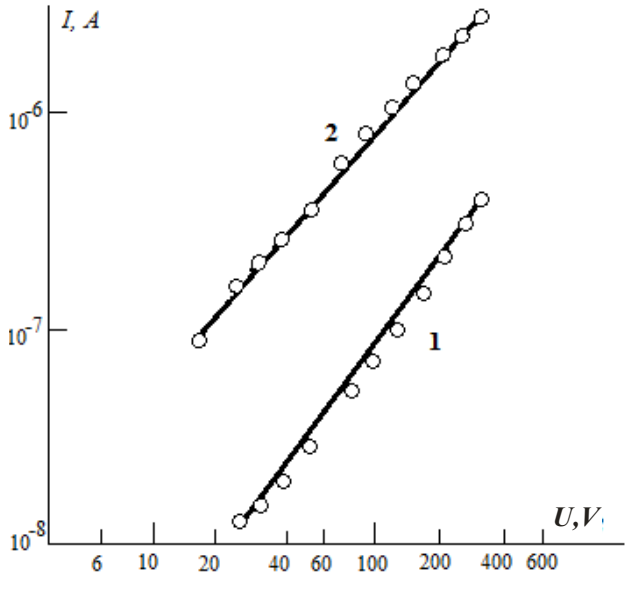


Fig. 2. The current-voltage characteristic of the sample SnO_2: curve 1 – in air, curve 2 – in vacuum. The precursor content is 10%; PVA - 1% (T = 293 K).

The Dark Current Temperature Dependence (DCTD), measured in a vacuum, is of an activa-

tion nature. That is, the current (and, hence, the electrical conductivity) increases with the temperature, obeying the exponential law (Fig. 3).

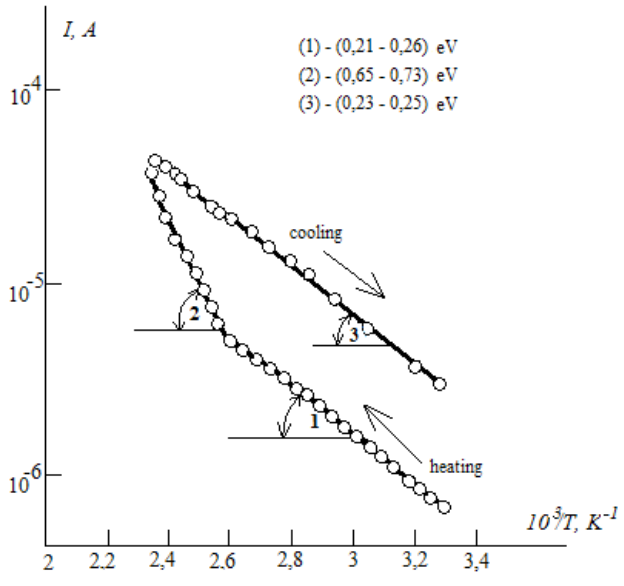


Fig. 3. The Dark Current Temperature Dependence of the film SnO_2, measured in vacuum (V = 500 B).

As it can be seen from Fig. 3, during the heating process in the low-temperature region, the current flow is controlled by donor levels with ionization energy (0.21-0.26) eV. According to the published data, they are doubly ionized vacancies of oxygen VO^{++} in the volume of SnO_2 films [8,9].

When the temperature of the sample (110-115) °C is reached, a sharp break is observed on the DCTD curve, and as the temperature increases further, the current grows with an activation energy E_a = (0.65-0.73) eV. The similar values of the conduction activation energy (0.72 eV) in the thin SnO_2 films, were registered by the authors [10], but without interpretation the nature of the corresponding defects.

The mentioned region may be associated with the water molecules desorption from the surface of the SnO_2 film.

The latter assumption is supported by the fact that the section with the indicated activation energy is absent on the DCTD curve measured during the cooling of the sample. On the DCTD curve, only the section with E_a = (0.23-0.25) eV, associated with the oxygen vacancies in the film volume, is observed throughout the temperature range [8,9].

The behavior of the DCTD curves measured in air (Fig. 4) in the temperature range up to +150 °C differs little from the DCTD curves measured in vacuum. However, in the region of higher temperatures (150 °C to 220 °C), steep regions with an activation energy (1.0 ± 1.4) eV appear on the dark current temperature dependence curves.

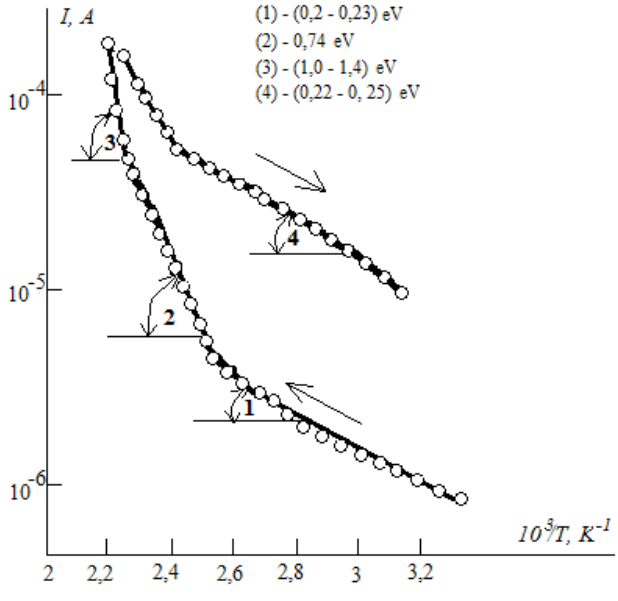


Fig. 4 The dark current temperature dependence of the SnO_2 film, measured in air (V = 500 B).

Perhaps these areas are due to dissociative adsorption of water on the surface of the tin dioxide layers [11-13].

According to the literature, tin dioxide sensors exhibit gas-sensitive properties in the temperature region above 300 °C [13]. The operating temperatures for sensors based on thin (and, in particular, nanostructured) SnO_2 films are much lower due to their porosity and the large effective surface area. The above given results of the Dark Current Temperature Dependencies make it possible to assume that these temperatures may be (110 ± 150) °C for the studied tin dioxide layers

Figure 5 shows the current-voltage characteristics of a SnO_2 sample measured at a temperature of +130 oC in an atmosphere of dry air (curve 1), and in the presence of water vapor (curve 2). It can be stated, that the film resistance in the wet

air atmosphere decreases several times as much. It is obvious, that a water vapor adsorbed on the tin dioxide surface leads to a resistance decrease.

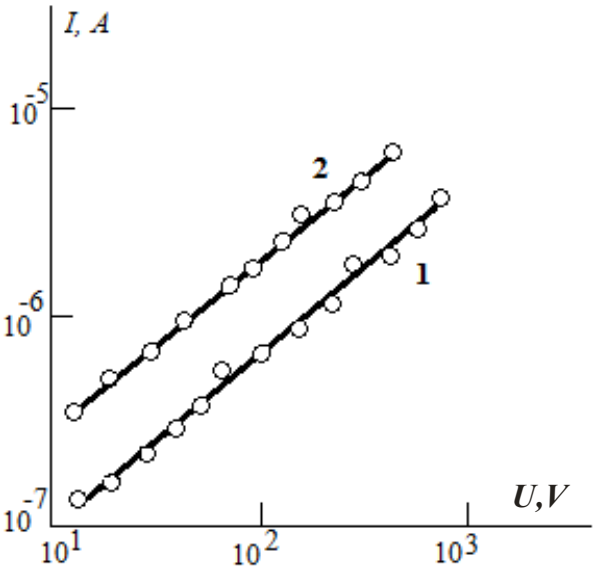


Fig. 5. The current-voltage characteristic of one of the SnO_2 films, measured at the temperature +130 °C in an atmosphere of dry air (1) and in the presence of water vapor (2).

At a high temperature on the SnO_2 microcrystal surface, the water molecule dissociates into the hydroxyl group OH^- and proton H^+ [14]. After the dissociation, the OH^- group is localized on the surface atom of tin, giving the electron to the conduction band of the semiconductor. The proton H^+ is captured by the O^- ion adsorbed on the surface, forming a neutral OH group. Thus, as a result of the adsorption process, the water molecules form two OH hydroxyl groups and hence the O^- ion disappears. This leads to an increase in conductivity. As the humidity level grows, the conductivity should also grow, due to the increase in the dissociative adsorption of water molecules [11], which is observed in our studies.

4. Conclusions

Thus, the conducted studies of the influence of the structuring additives concentration and humidity on the electrophysical properties of tin dioxide films made it possible to establish a number of corresponding features.

The increase in the interelectrode resistance of SnO_2 films with the corresponding polyvinyl acetate concentration growth increasing in the initial solution is due to the growth of porosity of the films under study with an increase in the amount of PVA.

A fragment with an activation energy E_a = (0.65-0.73) eV, apparently associated with the water molecules desorption, is observed on the DCTD curve measured in vacuum starting from (110-115) °C.

A decrease in tin dioxide films resistance in a wet atmosphere due to the dissociative adsorption of water molecules on the surface of SnO_2 layers has been established.

References

1. Granqvist, C.G. Transparent conductors as solar energy materials: A panoramic review. Sol. Energy Mat. Sol. Cells 2007, **91**, 1529-1598.
2. Handbook of Transparent Conductors, Ginley, D., Hosono, H., Paine, D. C. (Eds.), Springer US, 2011
3. Hyung-Sik Woo, Chan Woong Na and Jong-Heun Lee, Design of Highly Selective Gas Sensors via Physicochemical Modification of Oxide Nanowires: Overview, Sensors 16, 1531 (2016); doi:10.3390/s16091531
4. M. Batzill, U. Diebold. Review: The surface and materials science of tin oxide Progress in Surface Science 79 (2005) 47-154
5. Filevskaya L.N., Smyntyna V.A., Grinevich V.S. Morphology of nanostructured SnO_2 films prepared with polymers employment // Photoelectronics, 15, pp. 11-14 (2006).
6. B. Ulug, H.M. Türkdemir, A. Ulug, O. Büyükgüngör, M.B. Yücel, V.A. Smyntyna, V.S. Grinevich, L.N. Filevskaya. Structure, spectroscopic and thermal characterization of bis(acetylacetonato) dichlorotin(IV) synthesized in aqueous solution// Ukrainian chemical journal. –

2010. – Т. 76, №7. – С. 12-17.
7. Dhage S.R., Ravi V., Date S.K. Nonlinear I-V characteristics study of doped SnO_2. – Bulletin of Materials Science. 2004, **27**(1), P.43-45.
8. Синёв И.В. Температурная зависимость сопротивления тонкоплёночных резисторов на основе диоксида олова. – Дисс., Саратов, 2014, с.209.
9. Fonstad C.G., Rediker R.H. Electrical properties of high quality stannic oxide crystals. – Journal of Applied Physics, 2003, Vol. 42, № 7, P. 2911-2918.
10. Kalinina M.V. et al. Temperature dependence of the resistivity for metal-oxide semiconductors based on tin dioxide. – Glass physics and chemistry, 2003, Vol. 29, № 4, P. 422-427.
11. Гаман В.И., Физика полупроводниковых газовых сенсоров, Томск, «Издательство НТЛ» 2012.
12. Алмаев А.В., Сергейченко Н.В., Рудов Ф.В. Влияние уровня влажности на характеристики сенсоров водорода на основе тонких плёнок SnO_2. - Мат. XX Международной научно-практической конф., 2014, Томск, С. 315-317.
13. Рябцев С.В. Электрофизические и оптические свойства различных наноформ оксида олова: Автореф. канд. дисс., Воронеж, 2011, 32с.
14. Korotcenkov G., Brinzari V., Golovanov V., et al. Kinetics of gas response to reducing gases of SnO_2 films, deposited by spray pyrolysis // Sensors and Actuators. B. – 2004. – V. 98. – P. 41-45

This article has been received within April 2017

PACS 73.61.Le, 73.63.Bd

A. P. Chebanenko, L. M. Filevska, V. A. Smyntyna, N. S. Simanovich, V. S. Grinevych

THE HUMIDITY AND STRUCTURING ADDITIVES INFLUENCE ON ELECTROPHYSICAL CHARACTERISTICS OF TIN DIOXIDE FILMS

Summary

The structuring additive concentration and humidity influence on the electrophysical properties of tin dioxide films was studied. The growth of SnO_2 films interelectrode resistance with the growth of polyvinyl acetate concentration in the initial solution is due to the porosity increase caused by the PVA increase in the films under study. The section of dark current temperature dependence, in vacuum from 110 °C with an activation energy ~ 0.7 eV, is due to the water molecules desorption. The resistance decrease of tin dioxide films in a wet atmosphere due to the dissociative adsorption of water molecules on the SnO_2 layers surfaces has been established.

Keywords: tin dioxide, thin films, humidity.

PACS 73.61.Le, 73.63.Bd

А. П. Чебаненко, Л. Н. Филевская, В. А. Смынтына, Н. С. Симанович, В. С. Гриневич

ВЛИЯНИЕ ВЛАГИ И СТРУКТУРИРУЮЩЕЙ ДОБАВКИ НА ЭЛЕКТРОФИЗИЧЕСКИЕ ХАРАКТЕРИСТИКИ ПЛЕНОК ДИОКСИДА ОЛОВА

Резюме

Исследовано влияние концентрации структурирующей добавки и влажности на электрофизические свойства пленок диоксида олова. Возрастание межэлектродного сопротивления пле-

нок SnO_2 при увеличении концентрации поливинилацетата в исходном растворе обусловлено увеличением пористости исследуемых пленок с ростом количества ПВА. Участок ТЗТТ, в вакууме от 110 °С с энергией активации ~0,7 эВ обусловлен десорбцией молекул воды. Установлено снижение сопротивления пленок диоксида олова во влажной атмосфере, обусловленное диссоциативной адсорбцией молекул воды на поверхности слоев SnO_2.

Ключевые слова: диоксид олова, тонкие пленки, влажность.

PACS 73.61.Le, 73.63.Bd

А. П. Чебаненко, Л. Н. Филевська, В. А. Сминтина, Н. С. Сімановіч, В. С. Гріневіч

ВПЛИВ ВОЛОГИ І СТРУКТУРУЮЧОЇ ДОБАВКИ НА ЕЛЕКТРОФІЗИЧНІ ХАРАКТЕРИСТИКИ ПЛІВОК ДІОКСИДУ ОЛОВА

Резюме

Досліджено вплив концентрації структуруючої добавки і вологості на електрофізичні властивості плівок діоксиду олова. Зростання межелектродного опору плівок SnO_2 при збільшенні концентрації полівінілацетату в вихідному розчині обумовлено збільшенням пористості досліджуваних плівок із зростанням кількості ПВА. Ділянка ТЗТТ в вакуумі від 110 °С з енергією активації ~ 0,7 еВ обумовлена десорбцією молекул води. Встановлено зниження опору плівок діоксиду олова у вологій атмосфері, обумовлене дисоциативною адсорбцією молекул води на поверхні шарів SnO_2.

Ключові слова: діоксид олова, тонкі плівки, вологість.

UDC 539.182

A. V. Glushkov[1] , V. B. Ternovsky[2], A. V. Smirnov[1], A. A. Svinarenko[1]

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

GAUGE-INVARIANT RELATIVISTIC PERTURBATION THEORY APPROACH TO DETERMINATION OF ENERGY and SPECTRAL CHARACTERISTICS FOR HEAVY AND SUPERHEAVY ATOMS AND IONS: REVIEW

We reviewed an effective consistent ab initio approach to relativistic calculation of the spectra for multi-electron heavy and superheavy ions with an account of relativistic, correlation, nuclear, radiative effects is presented. The method is based on the relativistic gauge-invariant (approximation to QED) perturbation theory (PT) and generalized effective field nuclear model with using the optimized one-quasiparticle representation firstly in theory of the hyperfine structure for relativistic atom. The wave function zeroth basis is found from the Dirac equation with potential, which includes the core ab initio potential, the electric and polarization potentials of a nucleus. The correlation corrections of the high orders are taken into account within the Green functions method (with the use of the Feynman diagram's technique). There have taken into account all correlation corrections of the second order and dominated classes of the higher orders diagrams (electrons screening, particle-hole interaction, mass operator iterations). The magnetic inter-electron interaction is accounted in the lowest on α parameter (α is the fine structure constant), approximation, the self-energy part of the Lamb shift is taken effectively into consideration within the Ivanov-Ivanova non-perturbative procedure, the Lamb shift polarization part - in the generalized Uehling-Serber approximation with accounting for the Källen-Sabry $\alpha^2(\alpha Z)$ and Wichmann-Kroll $\alpha(\alpha Z)^n$ corrections.

1. Introduction

In last years a studying the spectra of heavy and superheavy elements atoms and ions is of a great interest for further development as atomic and nuclear theories (c.f.[1-8]). Theoretical methods used to calculate the spectroscopic characteristics of heavy and superheavy ions may be divided into three main groups: a) the multi-configuration Hartree-Fock method, in which relativistic effects are taken into account in the Pauli approximation, gives a rather rough approximation, which makes it possible to get only a qualitative idea on the spectra of heavy ions. b) The multiconfiguration Dirac-Fock (MCDF) approximation (the Desclaux program, Dirac package) [1,2] is, within the last few years, the most reliable version of calculation for multielectron systems with a large nuclear charge; in these calculations one- and two-particle relativistic effects are taken into account practically precisely. The calculation program of Desclaux is compiled with proper account of the finiteness of the nucleus size; however, a detailed description of the method of their investigation of the role of the nucleus size is lacking. In the region of small Z (Z is a charge of the nucleus) the calculation error in the MCDF approximation is connected mainly with incomplete inclusion of the correlation and exchange effects which are only weakly dependent on Z; c) In the study of lower states for ions with $Z \leq 40$ an expansion into double series of the PT on the parameters 1/Z, αZ (α is the fine structure constant) turned out to be quite useful. It permits evaluation of relative contributions of the different expansion terms: non-relativistic, relativistic, QED contributions as the functions of Z. Nevertheless, the serious problems in calculation of the heavy elements spectra are connected with developing new, high exact methods of account for the QED effects, in particular, the Lamb shift (LS), self-energy (SE) part of the Lamb shift, vacuum polarization (VP) contribution, correction on the nuclear finite size for heavy elements and its account for different spectral properties, including calculating the energies and constants of the hyperfine structure, derivatives of the 1-electron characteristics on nuclear

radius, nuclear electric quadrupole, magnetic dipole moments etc (c.f.[1-98]).

In present paper we review an effective initio approach to relativistic calculation of the spectra for multi-electron superheavy ions with an account of relativistic, correlation, nuclear, radiative effects is presented. The method is based on the relativistic gauge-invariant (approximation to QED) perturbation theory (PT) and generalized relativistic dynamical effective field nuclear model with using the optimized one-quasiparticle representation in theory of the hyperfine structure for relativistic systems [15-60].

The correlation corrections of the high orders are taken into account within the Green functions method (with the use of the Feynman diagram's technique). There have taken into account all correlation corrections of the second order and dominated classes of the higher orders diagrams (electrons screening, particle-hole interaction, mass operator iterations) [2,60-99]. The magnetic inter-electron interaction is accounted in the lowest on α^2 parameter, the LS polarization part - in the Uehling-Serber approximation, self-energy part of the LS is accounted effectively within the Ivanov-Ivanova non-perturbative procedure [5-8]. The expressions for the energies and constants of the hyperfine structure, deriviatives of 1-electron characteristics on nuclear radius, nuclear electric quadrupole, magnetic dipole moments Q etc are presented. As illustration some data for atom of hydrogen ^{1}H (test calculation) and superheavy H-like ion with nuclear charge Z=170, Li-like multicharged ions are listed.

2. Gauge-invariant relativistic many-body perturbation theory method for heavy ions

2.1. General Formalism

In atomic theory, a convenient field procedure is known for calculating the energy shifts ΔE of the degenerate states. Secular matrix M diagonalization is used. In constructing M, the Gell-Mann and Low adiabatic formula for ΔE is used. A similar approach, using this formula with the QED scattering matrix, is applicable in the relativistic theory. In contrast to the non-relativistic case, the secular matrix elements are already complex in the PT second order (first order of the inter-electron interaction). Their imaginary parts relate to radiation decay (transition) probability. The total energy shift of the state is usually presented as follows:

$$\Delta E = \mathrm{Re}\Delta E + \mathrm{i}\ \mathrm{Im}\Delta E, \qquad (1)$$

$$\mathrm{Im}\ \Delta E = -\Gamma/2, \qquad (2)$$

where Γ is interpreted as the level width, and the decay possibility P=Γ. The whole calculation of energies and decay probabilities of a non-degenerate excited state is reduced to calculation and diagonalization of the complex matrix M. To start with the Gell-Mann and Low formula it is necessary to choose the PT zero-order approximation. Usually, the one-electron Hamiltonian is used, with a central potential that can be treated as a bare potential in the formally exact QED PT. There are many well-known attempts to find the fundamental optimization principle for construction of the bare one-electron Hamiltonian (for free atom or atom in a field) or (what is the same) for the set of one-quasiparticle (QP) functions, which represent such a Hamiltonian [1-8]. As the bare potential, one usually includes the electric nuclear potential V_N and some parameterized screening potential V_C. The parameters of the bare potential may be chosen to generate the accurate eigen-energies of all many-QP states. In the PT second order the energy shift is expressed in terms of the two-QP matrix elements [6-8]:

$$V(1,2;4,3) = \sqrt{(2j_1+1)(2j_2+1)(2j_3+1)(2j_4+1)}\cdot \cdot(-1)^{j_1+j_2+j_3+j_4+m_1+m_2}\cdot \times\sum_{\lambda,\nu}(-1)^{\nu}\begin{bmatrix} j_1 \ldots\ldots j_3 \ldots \lambda \\ m_1 . - m_3 .. \nu \end{bmatrix}\begin{bmatrix} j_2 \ldots\ldots j_4 \ldots \lambda \\ m_2 . - m_4 .. \nu \end{bmatrix}(Q_\lambda^{Qul} + Q_\lambda^{Br}). \qquad (3)$$

Here Q_λ^{Qul} is corresponding to the Coulomb part of interaction (Q_λ^{B} -Breit part) :

$$Q_\lambda^{Qul} = \{R_\lambda(1243)S_\lambda(1243) + R_\lambda(\tilde{1}24\tilde{3})S_\lambda(\tilde{1}24 + R_\lambda(1\tilde{2}\tilde{4}3)S_\lambda(1\tilde{2}\tilde{4}3) + R_\lambda(\tilde{1}\tilde{2}\tilde{4}\tilde{3})S_\lambda(\tilde{1}\tilde{2}\tilde{4}\tilde{3})\}, \qquad (4)$$

where $R(1,2;4,3)$ is the radial integral of the Coulomb inter-QP interaction with large radial Dirac components; the tilde denotes a small Dirac com-

ponent; S_α is the angular multiplier (see details in Refs.[2-12]). To calculate all necessary matrix elements one must have the 1QP relativistic functions.

2.2 The Dirac-Kohn-Sham Relativistic Wave Functions

Usually, a multielectron atom is defined by a relativistic Dirac Hamiltonian(the a.u. used):

$$H = \sum_i h(r_i) + \sum_{i>j} V\left(r_i r_j\right). \qquad (5)$$

Here, *h(r)* is one-particle Dirac Hamiltonian for electron in a field of the finite size nucleus and *V* is potential of the inter-electron interaction. The relativistic inter electron potential is as follows [7,8]:

$$V\left(r_i r_j\right) = exp\left(i\omega_{ij} r_{ij}\right) \cdot \frac{\left(1 - \alpha_i \alpha_j\right)}{r_{ij}}, \qquad (6)$$

where α_{ij} is the transition frequency;α_i , α_j are the Dirac matrices. The Dirac equation potential includes the electric potential of a nucleus and exchange-correlation potential. One of the variants is the Kohn-Sham-like (KS) exchange relativistic potential, which is obtained from a Hamiltonian having a transverse vector potential describing the photons, is as follows [33]:

$$V_X[\rho(r), r] = V_X^{KS}(r) \cdot \{\frac{3}{2} \ln \frac{[\beta + (\beta^2+1)^{1/2}]}{\beta(\beta^2+1)^{1/2}} - \frac{1}{2}\}, \qquad (7)$$

$$\beta = [3\pi^2 \rho(r)]^{1/3} / c \qquad (8)$$

The corresponding correlation functional is [2,33]:

$$V_C[\rho(r), r] = -0.0333 \cdot b \cdot \ln[1 + 18.3768 \cdot \rho(r)^{1/3}], \qquad (9)$$

where *b* is the optimization parameter (see details in Refs. [2-4,9,10]).

One-particle wave functions are found from solution of the Dirac equation, which is written in the known two-component form:

$$\frac{\partial F}{\partial r} + (1+\chi)\frac{F}{r} - (\varepsilon + m - v)G = 0$$
$$\frac{\partial G}{\partial r} + (1-\chi)\frac{G}{r} + (\varepsilon - m - v)F = 0 \qquad (10)$$

Here we put the fine structure constant α=1, χ - the Dirac number. At large χ the radial functions F and G vary rapidly as:

$$F(r), G(r) \approx r^{\gamma - 1}$$
$$\gamma = \sqrt{\chi^2 - \alpha^2 Z^2} \qquad (11)$$

This involves difficulties in numerical integration of the equations for $r \to 0$. To prevent it, it is convenient to turn to new functions isolating main power dependence: $f = F^{\,1-|\chi|}$, $g = G^{\,1-|\chi|}$. The Dirac equation for *F* and *G* components are transformed as:

$$f' = -(\chi + |\chi|) f/r - \alpha Z V g - (\alpha Z E_{n\chi} + 2/\alpha Z) g$$
$$g' == (\chi - |\chi|) g/r - \alpha Z V f + \alpha Z E_{n\chi} \qquad (12)$$

Here the Coulomb units (C.u.) are used. In Coulomb units the atomic characteristics vary weakly with Z; E_n is one-electron energy without the rest energy. The boundary values of the correct solution are as:

$$g = (V(0) - E_{n\chi}) r\alpha\, Z/(2\chi + 1); \quad f = 1,\ \chi < 0$$
$$f = \left(V(0) - E_{n\chi} - 2/\alpha^2 Z^2\right)\alpha Z; \quad g = 1,\ \chi > 0 \qquad (13)$$

The condition $f, g \to 0$ at $r \to \infty$ determines the quantified energies E_n. The asymptotics of *f,g* at $r \to \infty$ are: f ,$g \sim \exp\left(-r/n^*\right)$ with effective quantum number $n^* = \sqrt{1/2|E_{n\chi}|}$.

2.3. Nuclear potential and charge density

Earlier there are calculated some characteristics of hydrogen-like ions with the nucleus in the form of a uniformly charged sphere; analogous calculations by means of an improved model were also made [2-8]. As in refs. [33-35] we use the relativistic mean-field (RMF) approach, which is an effective field theory for nuclei below an energy scale of 1GeV, separating the long- and intermediate-range nuclear physics from short-distance physics, involving, i.e., short-range correlations, nucleon form factors, vacuum polarization etc, which is absorbed into various terms and coupling constants. Usually one starts with a Lagrangian density describing Dirac spinor nucleons interacting via meson and photon fields. This leads then to the Dirac equation with the potential terms describing the nucleon dynamics and the Klein-Gordon-type equations involving nucleon-

ic currents and densities as source terms for mesons and the photon. In our approach we usually use the NL3-NLC (see details in refs. [33,38]), which is among the most successful parameterizations available. The resulted charge density is defined as:

$$\rho_c(R) = A\int dx \exp[-\mu(R-x)]\rho_p(x)\,, \quad (14a)$$

with the proton density ρ_p constructed from the RMF (A,μ are the numerical coefficients) and normalized to the charge number Z:

$$\int dR\rho_p(r) = Z\,. \quad (14b)$$

All corresponding model parameters are explained and given in refs. [33]. Another effective model approach to determine nuclear potential (the nuclear density distribution) is given by the known Fermi model. This model gives the following definition of the charge distribution $\rho(r)$:

$$\tilde{n}(r) = \tilde{n}_0 /\{1+\exp[(r-c)/a)]\}\,, \quad (15)$$

where the parameter a=0.523 fm; the parameter c is chosen by such a way that it is true the following condition for average-squared radius:

$$<r^2>^{1/2}=(0.836\cdot A^{1/3}+0.5700)\text{fm}. \quad (16)$$

We assume it as some zeroth approximation. Further the derivatives of various characteristics on R are calculated. They describe the interaction of the nucleus with outer electron; this permits recalculation of results, when R varies within reasonable limits. The Coulomb potential for the spherically symmetric density $\rho(r|R)$ is:

$$V_{nucl}(r|R) = -((1/r)\int_0^r dr' r'^2\rho(r'|R) + \int_r^\infty dr' r'\rho(r'|R) \quad (17)$$

It is determined by the following system of differential equations [7,8]:

$$V'nucl(r,R) = (1/r^2)\int_0^r dr' r'^2\rho(r',R) \equiv (1/r^2)y(r,R)$$

$$y'(r,R) = r^2\rho(r,R),$$

$$\rho'(r,R) = -8\gamma^{5/2} r/\sqrt{\pi}\exp(-\gamma r^2) = \quad (18)$$

$$= -2\gamma r\rho(r,R) = -\frac{8r}{\pi r^2}\rho(r,R)$$

with the corresponding boundary conditions.

2.4. QED corrections: Self-energy part of the Lamb shift and vacuum polarization correction

Procedure for an account of the radiative QED corrections is in details given in the refs. [2-4,8,33-35]. Regarding the vacuum polarization effect let us note that this effect is usually taken into account in the first PT theory order by means of the Uehling-Serber potential. This potential is usually written as follows (c.f.[2]):

$$U(r) = -\frac{2\alpha}{3\pi r}\int_1^\infty dt\exp(-2rt/\alpha Z)\bullet$$

$$(1+1/2t^2)\frac{\sqrt{t^2-1}}{t^2} \equiv -\frac{2\alpha}{3\pi r}C(g), \quad (19)$$

where $g = r/\alpha Z$. In calculation [7-9] it has been used more exact approach. The Uehling-Serber potential, determined as a quadrature (19) may be approximated with high precision by a simple analytical function. The use of new approximation of the Uehling-Serber potential permits one to decrease the calculation errors for this term down to 0.5 – 1%. It allows accounting for the Källen-Sabry $\alpha^2(\alpha Z)$ and Wichmann-Kroll $\alpha(\alpha Z)^n$ corrections [33-35]. Besides, using a simple analytical function form for approximating the Uehling-Serber potential allows its easy inclusion into the general system of differential equations. This system includes also the Dirac equations and the equations for matrix elements. A method for calculation of the self-energy part of the Lamb shift is based on an idea by Ivanov-Ivanova (c.f.[7,8]). In an atomic system the radiative shift and the relativistic part of the energy are, in. principle, determined by one and the same physical field. It may be supposed that there exists some universal function that connects the self-energy (SE) correction and the relativistic energy. The SE correction for the states of a hydrogen-like ion was presented by Mohr as:

$$E_{SE}(H|Z,nlj) = 0.027148\frac{Z^4}{n^3}F(H|Z,nlj) \quad (20)$$

The values of F are given at $Z = 10-110$, $nlj = 1s,2s,2p_{1/2},2p_{3/2}$. These results are modified here for the states $1s^2\,nlj$ of Li-like ions. It is supposed that for any ion with nlj electron over the core of closed shells the sought value may be presented in the form:

$$E_{SE}(Z,nlj) = 0.027148\frac{\xi^4}{n^3}f(\xi,nlj)\,(cm^{-1}) \quad (21)$$

The parameter $\xi = (E_R)^{1/4}$, E_R is the relativistic part of the bounding energy of the outer electron; the universal function $f(\xi, nlj)$ does not depend on the composition of the closed shells and the actual potential of the nucleus. The procedure of generalization for a case of Li-like ions with finite nucleus consists of the following steps [2,8,35]:

1). Calculation of the values E_R and ξ for the states *nlj* of H-like ions with the point nucleus (in accordance with the Zommerfeld formula);

2). Construction of approximating function *f* by the found reference Z and the appropriate *F*(H|*Z, nlj*);

3). Calculation of E_R and ξ for the states *nlj* of *Li*-like ions with the finite nucleus;

4). Calculation of E_{SE} for the sought states. The energies of the states of Li-like ions are calculated twice: with a conventional constant of the fine structure α=1/137and $\alpha'=\alpha/10^3$. The results of latter calculation are considered as non-relativistic. This permitted isolation of E_R,ξ. The above extrapolation method is more justified than using the known expansion on αZ parameter.

2.5. The hyperfine structure parameters

Energies of quadruple (W_q) and magnetic dipole ($W\mu$) interactions to define a hyperfine structure (HFS) are calculated as [32,35]:

$$W_q=[\Delta+C(C+1)]B,\quad W\mu=0{,}5\,AC,$$

$$\Delta=-(4/3)(4\chi-1)(I+1)/[i(I-1)(2I-1)],$$

$$C=F(F+1)-J(J+1)-I(I+1). \qquad (22)$$

Here *I* is a spin of nucleus, *F* is a full momentum of system, *J* is a full electron momentum. HFS constants are expressed through the standard radial integrals [2,8,35]:

$$A=\{[(4{,}32587)10^{-4}Z^2\chi g_I]/(4\chi^2-1)\}(RA)_{-2},$$

$$B=\{7.2878\ 10^{-7}\ Z^3Q/[(4\chi^2-1)I(I-1)\}\ (RA)_{-3}, \qquad (23)$$

Here g_I is the Lande factor, *Q* is a quadruple momentum of nucleus (in Barn); radial integrals are defined as follows:

$$(RA)_{-2}=\int_0^\infty drr^2F(r)G(r)U(1/r^2,R),$$
$$(RA)_{-3}=\int_0^\infty drr^2[F^2(r)+G^2(r)]U(1/r^3,R)\cdot \qquad (24)$$

For calculation of potentials of the hyperfine interaction $U(1/r^n,R)$, we solve the following differential equations [7,8]: $U(1/r^n,R)=-ny(r,R)/r^{n+1}$. The functions $dU(1/r^n,R)/dR$ are can be found by similar way. To obtain the corresponding value of *Q* one must combine the HFS constants data with the electric field gradient calculated in our approach too. The details of calculation are presented in [11,14, 17,18].

2.6. Correlation effects and construction of optimal 1-quasiparticle representation

The problem of the searching for the optimal one-electron representation is one of the oldest in the theory of multielectron atoms. One of the simplified recipes represents, for example, the DFT method (see [2,3]). Unfortunately, this method doesn't provide a regular refinement procedure in the case of the complicated atom with few quasiparticles (electrons or vacancies above a core of the closed electronic shells). We use the method [9,10]. For simplicity, let us consider now the one-quasiparticle atomic system. The multi-quasiparticle case doesn't contain principally new moments. In the lowest, second order, of the QED PT for the ΔE there is the only one-quasiparticle Feynman diagram a (fig.1), contributing the ImΔE (the radiation decay width).

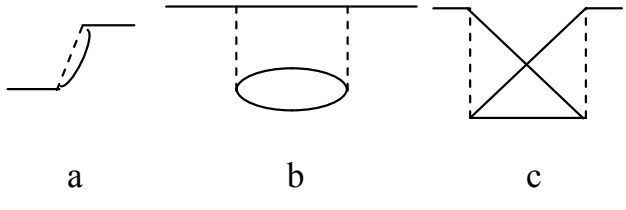


Figure 1. a: second other PT diagram contributing the imaginary energy part related to the radiation transitions; b and c: fourth order QED polarization diagrams.

In the next, the fourth order there appear diagrams, whose contribution into the ImΔE account for the core polarization effects. This

contribution describes collective effects and it is dependent upon the electromagnetic potentials gauge (the gauge non-invariant contribution). We examine the multielectron atom with one quasiparticle in the first excited state, connected with the ground state by the radiation transition. In the PT zeroth approximation one can use the one-electron bare potential:

$$V_N(r)+V_C(r), \qquad (25)$$

with $V_N(r)$ describing the electric potential of the nucleus, $V_C(r)$, imitating the interaction of the with the core of closed shells. The perturbation in terms of the second quantization representation reads as

$$-V_C(r)\ \psi^+(r)\ \psi(r)\ -\ j_\mu(x)\ A^\mu(x). \qquad (26)$$

The core potential $V_C(r)$ is related to the core electron density $\rho_C(r)$ in a standard way. The latter fully defines the one electron representation. Moreover, all the results of the approximate calculations are the functionals of the density $\rho_C(r)$. Here, the lowest order multielectron effects, in particular, the gauge dependent radiative contribution for the certain class of the photon propagator gauge is treating. This value is considered to be the typical representative of the electron correlation effects, whose minimization is a reasonable criteria in the searching for the optimal one-electron basis of the PT. Remember that the closeness of the radiation probabilities calculated with the alternative forms of the transition operator is commonly used as a criterion of the multielectron calculations quality. The imaginary part of the diagram a (fig.1) contribution has been presented previously as a sum of the partial contributions of α-*s* transitions from the initial state α to the final state *s* [10]:

$$\mathrm{Im}\Delta E_\alpha\,(\mathrm{a}) = \sum_s\ \mathrm{Im}\ \Delta E\ (\alpha\text{-}s;\ \mathrm{a}). \qquad (27)$$

Two fourth order polarization diagrams b,c (fig.1) should be considered further. The contributions being under consideration, are gauge-dependent, though the results of the exact calculation of any physical quantity must be gauge independent . All the non-invariant terms are multielectron by their nature. Let us take the photon propagator calibration as usually:

$$D = D_T + CD_L,$$

$$D_T = \delta_{\mu\nu}\ /\ (\ k_0^2\ -\ k^2\ ), \qquad (28)$$

$$D_L = -\ k_\mu k_\nu /\ (\ k_0^2 - k^2\ ).$$

Here C is the gauge constant; D_T represents the exchange of electrons by transverse photons, D_L that by longitudinal ones. One could calculate the contribution of the a,b,c diagrams (fig.1) into the Im ΔE taking into account both the D_T and D_L parts. The a diagram (fig.1) contribution into the Im ΔE related to the α-*s* transition reads as

$$\frac{1-\alpha_1\alpha_2}{r_{12}}\sin(\omega_{\alpha s}r_{12})\ \psi_\alpha(r_2)\ \psi_s(r_1), \qquad (29)$$

for $D = D_T$, and

$$-\frac{e^2}{8\pi}\int\int dr_1\,dr_2\ \psi_\alpha^+(r_1)\ \psi_s^+(r_2)\ \{[(1-\alpha_1 n_{12}\cdot \cdot\alpha_2 n_{12})/\ r_{12}\ ]\sin(\omega_{\alpha s}r_{12})+\omega_{\alpha s}\ .$$

$$(1+\alpha_1 n_{12}\alpha_2 n_{12})\times\cos(\omega_{\alpha s}r_{12})\}\ \psi_\alpha(r_2)\psi_s(r_1), \qquad (30)$$

for $D=D_L$, where $\omega\alpha_s$ is the α -*s* transition energy. According to the Grant theorem, the $D\mu\upsilon_L$ contribution vanishes, if the one-quasiparticle functions $\psi\alpha$, ψ_s satisfy the same Dirac equation. Nevertheless this term is to be retained when using the distorted waves approximation, for example. Another very important example represents the formally exact approach based on the bare Hamiltonian defined by its spectrum without specifying its analytic form [2,3]. Here the non-invariant contribution appears already in the lowest order. When calculating the forth order contributions some approximations are inevitable. These approximations have been formulated in Refs.[10], where the polarization corrections to the state energies have been considered.

Let us consider the direct polarization diagram b (fig.1) as an example. The final expression for the sought value looks as

$$\mathrm{Im}\,E_{ninv}(\alpha s\,|\,A_d) = -\frac{Ce^2}{4\pi}\iiint\int dr_1dr_2dr_3dr_4\sum(\frac{1}{\omega_{mn}+\omega_{\alpha_s}}+ \qquad (31)$$

$$+\frac{1}{\omega_{mn}-\omega_{\alpha_s}})\Psi_\alpha^+(r_1)\Psi_m^+(r_2)\Psi_s^+(r_3)\Psi_n^+(r_4)(1-\alpha_1\alpha_2)/r_{12}\cdot$$

$$\{[(\alpha_3\alpha_4 - (\alpha_3 n_{34})(\alpha_4 n_{34}))/r_{34} \cdot \sin[\omega_{\alpha_n}(r_{12}+r_{34}) + \omega_{\alpha_n} \cdot$$

$$\cos[\omega_{\alpha_n}(r_{12}+r_{34})](1+(\alpha_3 n_{34})(\alpha_4 n_{34}))]\} \cdot$$

$$\cdot \Psi_m(r_3)\Psi_\alpha(r_4)\Psi_n(r_2)\Psi_s(r_1)$$

Expression (31) can be represented in the form of sum of the following terms:

$$\sum \langle \alpha m | W_1 | ns \rangle \langle sn | W_2 | m\alpha \rangle / (\omega_{mn} \pm \omega_{\alpha s}) \quad (32)$$

With four different combinations of operators W_1 and W_2 (see [7-10]). In (31) it should be performed summation over the bound and upper continuum atomic states. To evaluate this sum, one can use the analytic relation between the atomic electron Fermi level and the core electron density $\rho_c(r)$, appropriate to the homogeneous nonrelativistic electron gas. Now the sum $\Sigma_{n>f,\, m<f}$ can be calculated analytically, its value becomes a functional of the core electron density. The resulting expression looks as the correction due to the additional nonlocal interaction of the active quasiparticle with the closed shells. Nevertheless, its calculation is reducible to the solving of the system of the ordinary differential equations (1-D procedure) [10]. The most important refinements can be introduced by accounting for the relativistic and the density gradient corrections to the Tomas- Fermi formula (see Refs. [2,3]). The same program is realized for other polarization diagrams. The minimization of the functional Im δE_{ninv} (b+c) leads to the integro-differential equation for the ρ_c (the Dirac-like equations for electron density). In result we obtain the optimal one-quasiparticle representation. In concrete calculation it is sufficient to use the simplified procedure, which is reduced to functional minimization using the variation of the parameter b in Eq.(9) [2,10]. Let us further to come back to the complex secular matrix M in the form:

$$M = M^{(0)} + M^{(1)} + M^{(2)} + M^{(3)}. \quad (33)$$

Here $M^{(0)}$ 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. It is usually 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 (33) one could have summarized all the contributions of the one -quasiparticle diagrams of all orders of the formally exact relativistic PT. The first two order corrections to $\mathrm{Re}\, M^{(2)}$ have been analyzed previously [2,5-9] using the Feynman diagrams technique. 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. An effective form for the two-particle polarizable operator has been presented in Ref. [2]; it looks as:

$$V^d_{pol}(r_1 r_2) = X \left\{ \int \frac{dr' \left(\rho_c^{(0)}(r')\right)^{1/3} \theta(r')}{|r_1 - r'| \cdot |r' - r_2|} - \right.$$

$$\left. - \int \frac{dr' \left(\rho_c^{(0)}(r')\right)^{1/3} \theta(r')}{|r_1 - r'|} \int \frac{dr'' \left(\rho_c^{(0)}(r'')\right)^{1/3} \theta(r'')}{|r'' - r_2|} \Big/ \left\langle \left(\rho_c^{(0)}\right)^{1/3} \right\rangle \right\},$$

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

$$\theta(r) = \left\{ 1 + \left[3\pi^2 \cdot \rho_c^{(0)}(r) \right]^{2/3} / c^2 \right\}^{1/2}, \quad (34)$$

where ρ_c^0 is the core electron density (without account for the quasiparticle), X is numerical coefficient, c is the light velocity. The similar approximate potential representation has been received for the exchange polarization interaction of quasiparticles. 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 others (look Refs. [2,3,7-10,33-35]). The calculation of all the radial integrals reduces to solving a system of differential equations with known boundary conditions at $r = 0$. Consider the master integral:

$$R^d_\lambda = \int\int\int dr_1 dr_2 dr_3 r_1^2 r_2^2 r_3^2 \rho_1(r_1)\tilde{U}_\lambda(r_1 r_3) \quad (35)$$
$$\rho_c^{1/3}(r_3)\tilde{U}_\lambda(r_3 r_2)\rho_2(r_2)$$

which enter the polarization contribution. This is the most complicated integral of a task. Let us note: $R^d = \lim_{r\to\infty} Y(r)$. According to [9], function $Y(r)$ can be found from solution of system of six differential equations with the boundary conditions:

$$Y_1' = (\rho_1 r^2 Z^{(1)}{}_\lambda - (\lambda+1)Y_1)/r,$$
$$Y_2' = (\rho_2 r^2 Z^{(1)}{}_\lambda - (\lambda+1)Y_2)/r,$$
$$Y_3' = (\rho_c^{1/3} r^2 Z^{(1)}{}_\lambda Z_\lambda^{(1)} - (2\lambda+1)Y_3)/r,$$
$$Y_4' = ((\rho_2 r^2 Y_3 + \rho_c^{1/3} Y_2 Z^{(1)}{}_\lambda Z_\lambda^{(2)} - (\lambda+1)Y_4)/r,$$
$$Y_5' = ((\rho_1 r^2 Y_3 + \rho_c^{1/3} Y_1 Z^{(1)}{}_\lambda Z_\lambda^{(2)} - (\lambda+1)Y_5)/r,$$
$$Y'(r) = (\rho_1 r^2 Y_4 + \rho_2 r^2 Y_5 + \rho_c^{1/3} r^2 Y_1 Y_2 Z_\lambda^{(2)}) Z_\lambda^{(2)}. \quad (36)$$

A complete system of equations also includes equations for the modified Bessel functions $Z^{(i)}$ and for 1QP radial functions (see [2-8]).

3 Some illustration results and conclusion

In table 1 we present the experimental [8,32-25] an theoretical (our test calculation) results for hyperfine splitting energies for 1s, 2s levels of hydrogen atom. There is physically reasonable agreement between theory and experiment.

Table 1

Experimental and theoretical data for HFS energies for 1s, 2s H-atom levels

Electron term Quantum numbers of total moment	Experiment Δν(F,F'), MHz ΔE(F,F'), 10^{-3} cm^{-1}	Theory [13] Δν(F,F'), MHz ΔE(F,F'), 10^{-3} cm^{-1}
1s $^2S_{1/2}$ (1,0)	1420,406 47, 379	1419,685 47, 355
2s $^2S_{1/2}$ (1,0)	177,557 5, 923	177,480 5, 920

In table 2 there are listed the results of calculation for the hyperfine structure parameters (plus derivatives of the energy contribution on nuclear radius) for the superheavy H-like ion with nuclear charge Z=170. We have used the denotations [7,8]:

$A=10^8 A/Z^3 g_I,(eV);$

$DA=(10^{-2}/Z^4 g_I)(\partial A/\partial R),\ (eV/cm);$

$B=(10^7 BI(2I-1))/Z^3 Q,\ (eV/Barn);$

$DB=[(10^{-3} I(2I-1))/Z^4 Q](\partial B/\partial R),$ *(eV/Barn cm)*;

$U=-(10^4/Z^4)\langle U(r,R)\rangle,\ (eV);$

$DU=(10^{-1}/Z^5)(\partial\langle U(r,R)\rangle/\partial R),\ (eV/cm);.$

$DV=[10^{-8}/Z^3](\partial\langle V\rangle/\partial R),\ (eV/cm);$

Table 2

Parameters of one-electron states for H-like ion with Z=170 (data from [8,35])

	$1s_{1/2}$	$2s_{1/2}$	$2p_{1/2}$	$2p_{3/2}$
A	4337	831	3867	1,59
DA	1039	228	941	0,0001
B	9091	1897	8067	0,07
DB	7245	1557	6405	0,0008
DV	1255	273	1108	0,0011
U	1453	282	1301	1,31
DU	2343	503	2071	0,0015
	$1s_{1/2}$	$3s_{1/2}$	$3p_{1/2}$	$3p_{3/2}$
A	4337	207	322	0,615
DA	1039	56,8	84,0	0,0001
B	9091	475	707	0,04
DB	7245	395	574	0,0003
DV	1255	67,7	98,3	0,0005
U	1453	69,3	109	0,62
DU	2343	127	185	0,0007

In table 3 there are listed the nuclear corrections into energy of the low transitions for Li-like ions.

Table 3

Nuclear finite size corrections into energy (cm^{-1}) for Li-like ions and values of the effective radius of nucleus (10^{-13} cm)

Z	$2s_{1/2}$-$2p_{1/2}$	$2s_{1/2}$-$2p_{3/2}$	R
20	- 15,1	- 15,5	3,26
41	- 659,0	- 670,0	4,14
69	- 20 690,0	- 21 712,0	4,93
79	- 62 315,0	- 66 931,0	5,15
92	- 267 325,0	- 288 312,0	5,42

The calculation showed also that a variation of the nuclear radius on several persents could lead to changing the transition energies on dozens of thousands $10^3 cm^{-1}$. In [8,32,35] there are listed the results of calculating the constants of the hyperfine interaction: the electric quadruple constant *B*, the magnetic dipole constant *A* with inclusion of nuclear finiteness and the Uehling-Serber potential for some Li-like ions. In table 4 data on the HFS constants for lowest excited states of Li-like ions are listed. Similar data for other states were listed earlier (see ref. [8,32,34]), but there another model for a charge distribution in a nucleus and method of treating the QED corrections were used.

Table 4.

Constants of the hyperfine electron-nuclear interaction: $A=Z^3 g_I \frac{}{A}_1 cm^{-1}$, $B=\frac{Z^3 Q}{I(2I-1)} \frac{}{B} cm^{-}$

nlj	*Z*	20	79	92
2s	$\frac{}{A}$	93 –03	215 -02	314 -02
3s	$\frac{}{A}$	26 –03	63 –03	90 –03
$2p_{1/2}$	$\frac{}{A}$	25 –03	71 –03	105 –02
$3p_{1/2}$	$\frac{}{A}$	81 –04	20 –03	31 –03
$2p_{3/2}$	$\frac{}{A}$	50 –04	71 –04	72 –04
	$\frac{}{B}$	9 –04	15 –04	17 –04
$3p_{3/2}$	$\frac{}{A}$	13 –04	21 –04	22 –04
	$\frac{}{B}$	31 –05	55–05	62 –05
$3d_{3/2}$	$\frac{}{A}$	88 –05	11 –04	12 –04
	$\frac{}{B}$	51 –06	10 –05	11 –05
$3d_{5/2}$	$\frac{}{A}$	36 –05	50 –05	52 –05
	$\frac{}{B}$	21 –06	39 –06	40 –06

References

1. Grant I.P., Relativistic Quantum Theory of Atoms and Molecules. – Oxford, 2008. – 650 p.
2. Glushkov A.V., Relativistic Quantum Theory. Quantum, mechanics of Atomic Systems. – Odessa: Astroprint, 2008. – 700 p.
3. Glushkov A.V., Relativistic and correlation effects in spectra of atomic systems.-Odessa: Astroprint. – 2006. – 400 p.
4. Glushkov A.V., Atom in electromagnetic field. – Kiev: KNT, 2005. – 450P.
5. Ivanov L.N.,Ivanova E.P., Extrapolation of atomic ion energies by model potential method: Na-like spectra/ // Atom. Data Nucl. Data Tab. – 1999. – Vol.24. – P. 95-121.
6. Ivanov L.N., Letokhov V.S., Autoionization states of multielectron atoms// Com. Of Modern Phys. D. Atom. and Mol.Phys. –1995. –Vol. 4. – P. 169-184.
7. 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, Mg-like and Ne-like ions // Phys.Scripta –1985. – Vol. 32, № 4. – P. 513-522.

8. Ivanova E.P., Ivanov L.N., Aglitsky E.V., Modern Trends in Spectroscopy of multi-charged Ions// Phys.Rep. – 1998. – Vol. 166, № 6. – P. 315-390.
9. 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.58-160.
10. 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.
11. Ivanov L.N., Ivanova E.P., Knight L., Energy approach to consistent QED theory for calculation of electron-collision strengths// Phys. Rev.A. – 1993. – Vol. 48. – P. 4365-4374.
12. 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.
13. 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.
14. 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.
15. Glushkov A.V., Khetselius O., Svinarenko 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. – 51 p.
16. 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.
17. Glushkov A.V., Khetselius O.Yu., Prepelitsa G., 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 International Geometry Center". – 2013. – Vol. 6, N 1. – P. 43-48.
18. 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.
19. Malinovskaya S.V., Glushkov A.V., Khetselius O.Yu., Lopatkin Yu., Loboda A.V., Svinarenko 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, N 2. – P. 288-296.
20. Malinovskaya S.V., Glushkov A.V., Khetselius O.Yu., Svinarenko A.A., Mischenko E.V., Florko T.A., Optimized 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, N 14. – P. 3325-3329.

21. Glushkov A.V., Khetselius O.Y., Malinovskaya S.V., Spectroscopy of cooperative laser-electron nuclear effects in multiatomic molecules// Molec. Phys. (UK). – 2008. – Vol. 106. – N 9-10. – P. 1257-1260.
22. 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.
23. 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.
24. Glushkov A.V., Effective quasi-particle valence hamiltonian of molecules in the comprehensive semi-empirical theory// Sov. Journ. Struct. Chem. – 1998. – Vol. 29, N 4. – P. 3-9.
25. Glushkov A.V., Loboda A.V., Gurnitskaya E., Svinarenko A., QED theory of radiation emission and absorption lines for atoms in a strong laser field//Phys. Scripta. – 2009. – T. 135. – P. 014022.
26. 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.
27. 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.
28. 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.
29. 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.
30. 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. – N 8. – P. 1717-1727.
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, N 14. – P. 3473-3481.
32. 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.
33. 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.
34. 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 com-

plex energy and mean-field nuclear potential// Frontiers in Quantum Methods and Applications in Chem. and Physics. Ser.: Progress in Theor. Chemistry and Phys., Eds. M. Nascimento, J.Maruani, E.Brändas, G. Delgado-Barrio (Springer). – 2015. – Vol. 29. – P. 197-217.
35. 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.Brändas, G.Delgado-Barrio (Springer). – 2015. – Vol. 29. – P. 55-76.
36. 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.
37. 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.
38. 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.
39. 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.
40. Ternovsky V.B., Glushkov A.V., Zaichko P., 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.
41. 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.
42. 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.
43. Buyadzhi V.V., Zaichko P.A., Gurskaya M., Kuznetsova A.A., Ponomarenko E.L., Ternovsky E.,Relativistic theory of excitation and ionization of Rydberg atoms in a Black-body radiation field//J. Phys.: Conf. Series.-2017.-Vol.810.-P. 012047.
44. Glushkov A.V., Khetselius O.Y., Brusentseva S.V., Zaichko P.A., Ternovsky V.B., Studying interaction dynamics of chaotic systems within a non-linear prediction method: application to neurophysiology// Advances in Neural Networks, Fuzzy Systems and Artificial Intelligence, Series: Recent Advances in Computer Engineering, Ed. J.Balicki.-2014.-Vol.21.-P.69-75.
45. Glushkov A.V., Svinarenko A.A., Buyadzhi V.V., Zaichko P., Ternovsky V., Chaos-geometric attractor and quantum neural networks approach to simulation chaotic evolutionary dynamics during perception process// Advances in Neural Networks, Fuzzy Systems and Artificial Intelligence, Series: Recent Advances in Computer Engineering, Ed. J.Balicki.-2014.-Vol.21.-P.143-150.
46. 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.

47. 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
48. Glushkov A.V., Khetselius O.Yu., Lopatkin Y., Florko T.A., Kovalenko O., Mansarliysky V., Collisional shift of hyperfine line for rubidium in an atmosphere of the buffer inert gas//J. Phys.:Conf.Series.-2014.-Vol.548.-P.012026
49. 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.
50. 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.
51. 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.
52. 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.
53. 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.
54. Khetselius O., Hyperfine structure of atomic spectra.-Odessa: Astroprint, 2008.-210P.
55. Khetselius O.Yu., Hyperfine structure of radium// Photoelectronics.-2005.-N14.-P.83-85.
56. Khetselius O., Spectroscopy of cooperative electron-gamma-nuclear processes in heavy atoms: NEET effect// J. Phys.: Conf. Ser.-2012.- Vol.397.-P.012012
57. 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.
58. 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.
59. 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.
60. 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.
61. Glushkov A.V., Khetselius O.Y., Brusentseva S.V., Zaichko P.A., Ternovsky V.B., Studying interaction dynamics of chaotic systems within a non-linear prediction method: application to neurophysiology// Advances in Neural Networks, Fuzzy Systems and Artificial Intelligence, Ser: Recent Adv. in Computer Engineering, Ed. J.Balicki.-2014.-Vol.21.-P.69-75.
62. Khetselius O.Yu., Quantum Geometry: New approach to quantization of the quasistationary states of Dirac equation for super heavy ion and calculating hy-

per fine structure parameters// Proc. Int. Geometry Center.-2012.-Vol.5,№ 3-4.-P.39-45.
63. 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.
64. 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.
65. 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.
66. 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.
67. Khetselius O.Yu., Hyperfine structure of energy levels for isotopes 73Ge, 75As, 201Hg// Photoelectronics.-2007.-N 16.-P. 129-132.
68. 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.-N 3.-P. 35-39.
69. Khetselius O.Y., Gurnitskaya E.P., Sensing the hyperfine structure and nuclear quadrupole moment for radium// Sensor Electr. and Microsyst. Techn.-2006.-N 2.-P. 25-29.
70. 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.-N 3.-P. 10-15.
71. Sukharev D.E., Khetselius O.Yu., Dubrovskaya Yu.V., Sensing strong interaction effects in spectroscopy of hadronic atoms// Sensor Electr. and Microsyst. Techn.-2009.-N 3.-P. 16-21.
72. Glushkov A.V., Khetselius O.Yu., Kuzakon V., Prepelitsa G.P., Solyanikova E.P., Svinarenko A., Modeling of interaction of the non-linear vibrational systems on the basis of temporal series analyses (application to semiconductor quantum generators)// Dynamical Systems-Theory and Applications.-2011.-BIF110.
73. Svinarenko A.A., Nikola L. V., Prepelitsa G., 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.
74. 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
75. 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.
76. 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.
77. 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.
78. 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.
79. 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.
80. 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, N 6. - P. 889-893.
81. 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, N 1. - P. 195-204.
82. 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
83. 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.
84. Glushkov A.V., Ambrosov S.V., Loboda A.V., Gurnitskaya E.P., Khetselius O.Yu., QED calculation of heavy multicharged ions with account for the correlation, radiative and nuclear effects// Recent Advances in Theor. Phys. and Chem. Systems.-2006.-Vol.15.-P.285-300.
85. 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.
86. 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 shileding approximation// Sensor Electr. and Microsyst. Techn.-2007.-N2.-P.9-13
87. 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.
88. Glushkov A.V., Bunyakova Yu.Ya., Zaichko P., Geometry of Chaos: Consistent combined approach to treating chaotic dynamics atmospheric pollutants and its forecasting// Proc. International Geometry Center".-2013.-Vol.6, N3.-P.6-14.
89. 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.
90. 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.
91. 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.
92. Serbov N.G., Glushkov A.V., Bunyakova Yu.Ya., Prepelitsa G.P., Svinarenko A.A., Sensing the kinetical features of energy exchange in mixture CO_2-N_2-H_20 of atmospheric gases under interacting with laser radiation// Sensor Electr. and Microsyst. Techn.-2006.-N4.-P.20-22.
93. Glushkov A.V., Khetselius O.Y., Bun-

yakova Yu.Ya., Prepelitsa G.P., Solyanikova E.P., Serga E., Non-linear prediction method in short-range forecast of atmospheric pollutants: low-dimensional chaos// Dynamical Systems - Theory and Applications (Lodz).-2011.-P.39-44 (LIF111).
94. Khetselius O.Yu., Forecasting evolutionary dynamics of chaotic systems using advanced non-linear prediction method// Dynamical Systems – Theory and Applications, Eds. J. Awrejcewicz, M. Kazmierczak, P. Olejnik, J, Mrozowski.-2013.-Vol.1.-P.145-152.
95. Glushkov A.V., Kuzakon V.M., Ternovsky V.B., Buyadzhi V.V., Dynamics of laser systems with absorbing cell and backward-wave tubes with elements of a chaos// Dynamical Systems – Theory and Applications, Eds. J. Awrejcewicz, M. Kazmierczak, P. Olejnik, J, Mrozowski.-2013.-Vol.T1.-P.461-466.
96. Bunyakova Yu.Ya., Khetselius O.Yu., Non-linear prediction statistical method in forecast of atmospheric pollutants// Proc. of 8th International Carbon Dioxide Conference.-2009.-P.T2-098.
97. Glushkov A.V., Khetselius O., 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.
98. 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.
99. 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.

This article has been received in May 2017

UDC 539.182

A. V. Glushkov, V. B. Ternovsky, A. V. Smirnov, A. A. Svinarenko

GAUGE-INVARIANT RELATIVISTIC PERTURBATION THEORY APPROACH TO DETERMINATION OF ENERGY and SPECTRAL CHARACTERISTICS FOR HEAVY AND SUPERHEAVY ATOMS AND IONS: REVIEW

Summary

We reviewed an effective consistent ab initio approach to relativistic calculation of the spectra for multi-electron heavy and superheavy ions with an account of relativistic, correlation, nuclear, radiative effects is presented. The method is based on the relativistic gauge-invariant (approximation to QED) perturbation theory (PT) and generalized effective field nuclear model with using the optimized one-quasiparticle representation firstly in theory of the hyperfine structure for relativistic atom. The wave function zeroth basis is found from the Dirac equation with potential, which includes the core ab initio potential, the electric and polarization potentials of a nucleus. The correlation corrections of the high orders are taken into account within the Green functions method (with the use of the Feynman diagram's technique). There have taken into account all correlation corrections of the second order and dominated classes of the higher orders diagrams (electrons screening, particle-hole interaction,

mass operator iterations). The magnetic inter-electron interaction is accounted in the lowest on α parameter (α is the fine structure constant), approximation, the self-energy part of the Lamb shift is taken effectively into consideration within the Ivanov-Ivanova non-perturbative procedure, the Lamb shift polarization part - in the generalized Uehling-Serber approximation with accounting for the Källen-Sabry $\alpha^2(\alpha Z)$ and Wichmann-Kroll $\alpha(\alpha Z)^n$ corrections.

Keywords: Relativistic perturbation theory, Heavy ions, Relativistic energy formalism

УДК 539.182

А. В. Глушков, В. Б. Терновский, А. В. Смирнов, А. А. Свинаренко

МЕТОД КАЛИБРОВОЧНО-ИНВАРИАНТНОЙ РЕЛЯТИВИСТСКОЙ ТЕОРИИ ВОЗМУЩЕНИЙ К ОПРЕДЕЛЕНИЮ ЭНЕРГЕТИЧЕСКИХ И СПЕКТРАЛЬНЫХ ХАРАКТЕРИСТИК ТЯЖЕЛЫХ И СВЕРХТЯЖЕЛЫХ АТОМОВ И ИОНОВ: ОБЗОР

Резюме

В работе обзорно изложены основы эффективного, последовательного ab initio подхода к релятивистскому вычислению спектров многоэлектронных тяжелых и сверхтяжелых ионов с учетом релятивистских, корреляционных, ядерных, радиационных эффектов. Метод основан на релятивистской калибровочно-инвариантной (КЭД) теории возмущений, обобщенной эффективной полевой модели ядра с использованием оптимизированного одноквазичастичного представления впервые в теории сверхтонкой структуры спектра релятивистского атома. Базис волновых функций нулевого приближения определяется решениями Dirac уравнения с потенциалом, который включает в себя самосогласованный ab initio электронный потенциал, электрический и поляризационный потенциалы ядра. Корреляционные поправки высших порядков учитываются в рамках метода функций Грина (с использованием техники диаграмм Feynman). Учтены все корреляционные поправки второго порядка и доминирующие классы диаграмм высших порядков (экранирование электронов, взаимодействие частицы с дыркой, итерации массового оператора). Магнитное межэлектронное взаимодействие учитывается в низшем по параметру α (α - постоянная тонкой структуры)приближении, собственно-энергетическая часть лэмбовского сдвига эффективно учитывается в рамках обобщенной непертурбативной процедуры Ivanov-Ivanova, эффект поляризации вакуума лэмбовского сдвига - в приближении Uehling-Serber с учетом поправок Källen-Sabry $\alpha^2(\alpha Z)$ и Wichmann-Kroll $\alpha(\alpha Z)^n$ (Z – заряд ядра).

Ключевые слова: Калибровочно-инвариантная релятивистская теория возмущений, Тяжелые ионы, Релятивистский энергетический формализм

УДК 539.182

О. В. Глушков, В. Б. Терновський, А. В. Смірнов, А. А. Свинаренко

МЕТОД КАЛІБРУВАЛЬНО-ІНВАРІАНТНОЇ РЕЛЯТИВІСТСЬКОЇ ТЕОРІЇ ЗБУРЕНЬ ДО ВИЗНАЧЕННЯ ЕНЕРГЕТИЧНИХ І СПЕКТРАЛЬНИХ ХАРАКТЕРИСТИК ВАЖКИХ І НАДВАЖКИХ АТОМІВ ТА ИОНОВ: ОГЛЯД

Резюме

В роботі оглядово викладені основи ефективного, послідовного ab initio підходу до релятивістського обчислення спектрів багатоелектронних важких і надважких іонів з урахуванням

релятивістських, кореляційних, ядерних, радіаційних ефектів. Метод заснований на релятивістської калібрувально-інваріантної (КЕД) теорії збурень, узагальненої ефективної польової моделі ядра з використанням оптимізованого одноквазічастинкового представлення вперше в теорії надтонкої структури спектру релятивістського атома. Базис хвильових функцій нульового наближення визначається рішеннями Dirac рівняння з потенціалом, який включає в себе самоузгоджений ab initio електронний потенціал, електричний і поляризаційний потенціали ядра. Кореляційні поправки вищих порядків враховуються в рамках методу функцій Гріна (з використанням техніки діаграм Feynman). Враховано всі кореляційні поправки другого порядку і домінуючі класи діаграм вищих порядків (екранування електронів, взаємодія частинки з діркою, ітерації масового оператора). Магнітна міжелектронна взаємодія враховується в нижчому за параметром α (α - стала тонкої структури) наближенні, власне-енергетична частина лембовського зсуву ефективно враховується в рамках узагальненої непертурбативної процедури Ivanov-Ivanova, ефект поляризації вакууму лембовського зсуву - в наближенні Uehling-Serber з урахуванням поправок Källen-Sabry $\alpha^2(\alpha Z)$ та Wichmann-Kroll $\alpha(\alpha Z)^n$ (Z – заряд ядра).

Ключові слова: Калібрувально-інваріантна релятивістська теорія збурень, Важкі іони, Релятивістський енергетичний формалізм

UDC 541.13

O. Yu. Khetselius, A. V. Glushkov, V. V. Buyadzhi, Yu. Ya. Bunyakova

Odessa State Environmental University, 15, Lvovskaya str., Odessa, Ukraine
E-mail: buyadzhivv@gmail.com

NEW NONLINEAR CHAOS-DYNAMICAL ANALYSIS OF ATMOSPHERIC RADON ^{222}RN CONCENTRATION TIME SERIES FROM BETA PARTICLES ACTIVITY DATA OF RADON MONITORS

The work is devoted to the development of the theoretical foundations of new universal complex chaos-dynamical approach to analysis and prediction of the atmospheric radon ^{222}Rn concentration changing from beta particles activity data of radon monitors (with pair of the Geiger-Müller counters). The approach presented consistently includes a number of new or improved methods of analysis (correlation integral, fractal analysis, algorithms of average mutual information, false nearest neighbors, Lyapunov exponents, surrogate data, non-linear prediction schemes, spectral methods, etc.) to solve problems quantitatively complete modeling and analysis of temporal evolution of the atmospheric radon ^{222}Rn concentration . There are firstly received data on topological and dynamical invariants for the time series of the ^{222}Rn concentration, discovered a deterministic chaos phenomenon using detailed data of measurements of the radon concentrations at SMEAR II station of the Finnish Meteorological Institute.

1. Introduction

At present time one of the extremely important and too complex areas of elements, systems and devices physics and sensor electronics is study of regular and chaotic dynamics dynamics of nonlinear processes in the different classes of quantum, quantum-generating systems and devices and quantum (atomic-molecular systems in an external electromagnetic field) [1-20]. It is worth to mention fulfilled by our group numerous studying of dynamics of the different quantum systems in external electromagnetic field, which has the features of the random, stochastic kind and its realization does not require the specific conditions.

The importance of studying a phenomenon of stochasticity or quantum chaos in dynamical systems is provided by a whole number of technical applications, including a necessity of understanding chaotic features in a work of different electronic devices and systems. New field of investigations of the quantum and other systems has been provided by a great progress in a development of a chaos theory methods [1-12]. In previous our papers [5-20] we have given a review of new methods and algorythms to analysis of different systems of quantum physics, electronics and photonics and used the nonlinear method of chaos theory and the recurrence spectra formalism to study quantum stochastic futures and chaotic elements in dynamics of atomic, molecular, nuclear systems in an free state and an external electromagnetic field, atmospheric and even environmental systems [21-71]. There were discovered non-trivial manifestations of a chaos phenomenon.

The work is devoted to the development of the theoretical foundations of new universal complex chaos-dynamical approach to analysis and prediction of the atmospheric radon ^{222}Rn concentration changing from beta particles activity data of radon monitors (with pair of the Geiger-Müller counters). The approach presented consistently includes a number of new or improved methods of analysis (correlation integral, fractal analysis, algorithms, average mutual information, false nearest neighbors, Lyapunov exponents, surrogate data, non-linear prediction, spectral methods, etc.) to solve problems quantitatively complete modeling and analysis of temporal evolution of the atmospheric radon ^{222}Rn concentration . There are firstly received data on topological and dynamical invariants for the time series of the ^{222}Rn concentration, discovered a deterministic chaos phenomenon using detailed data of measurements of the radon concentrations at SMEAR

II station of the Finnish Meteorological Institute (see details in Refs. [72-75]).

2. Universal chaos-dynamical approach in analysis of chaotic dynamics of the radon concentration time series

As many blocks of the presented approach have been developed earlier and are needed only to be reformulated regarding the problem studied in this paper, here we are limited only by the key moments following to Refs. [5-20]. Let us formally consider scalar measurements $s(n) = s(t_0 + n\Delta t) = s(n)$, where t_0 is the start time, Δt is the time step, and is n the number of the measurements. Further it is necessary to reconstruct phase space using as well as possible information contained in the s(n). Such a reconstruction results in a certain set of d-dimensional vectors y(n) replacing the scalar measurements. Packard et al. introduced the method of using time-delay coordinates to reconstruct the phase space of an observed dynamical system. The direct use of the lagged variables $s(n + \tau)$, where τ is some integer to be determined, results in a coordinate system in which the structure of orbits in phase space can be captured. Then using a collection of time lags to create a vector in d dimensions,

$$\mathbf{y}(n) = [s(n), s(n+\tau), s(n+2\tau), \ldots, s(n+(d-1)\tau)], \quad (1)$$

the required coordinates are provided. In a nonlinear system, the $s(n + j\tau)$ are some unknown nonlinear combination of the actual physical variables that comprise the source of the measurements. The dimension d is called the embedding dimension, d_E. Aany time lag will be acceptable is not terribly useful for extracting physics from data. If τ is chosen too small, then the coordinates $s(n + j\tau)$ and $s(n + (j + 1)\tau)$ are so close to each other in numerical value that they cannot be distinguished from each other. Similarly, if τ is too large, then $s(n + j\tau)$ and $s(n + (j + 1)\tau)$ are completely independent of each other in a statistical sense. Also, if τ is too small or too large, then the correlation dimension of attractor can be under- or overestimated respectively [3]. It is therefore necessary to choose some intermediate (and more appropriate) position between above cases. First approach is to compute the linear autocorrelation function

$$C_L(\delta) = \frac{\frac{1}{N}\sum_{m=1}^{N}[s(m+\delta)-\bar{s}]\,[s(m)-\bar{s}]}{\frac{1}{N}\sum_{m=1}^{N}[s(m)-\bar{s}]^2}, \qquad \bar{s} = \frac{1}{N}\sum_{m=1}^{N} s(m) \quad (2)$$

and to look for that time lag where $C_L(\delta)$ first passes through zero. This gives a good hint of choice for τ at that $s(n + j\tau)$ and $s(n + (j + 1)\tau)$ are linearly independent. However, a linear independence of two variables does not mean that these variables are nonlinearly independent since a nonlinear relationship can differs from linear one. It is therefore preferably to utilize approach with a nonlinear concept of independence, e.g. the average mutual information. Briefly, the concept of mutual information can be described as follows. Let there are two systems, A and B, with measurements a_i and b_k. The amount one learns in bits about a measurement of a_i from measurement of b_k is given by arguments of information theory [2,8,9]

$$I_{AB}(a_i, b_k) = \log_2\left(\frac{P_{AB}(a_i, b_k)}{P_A(a_i)P_B(b_k)}\right), \quad (3)$$

where the probability of observing a out of the set of all A is $P_A(a_i)$, and the probability of finding b in a measurement B is $P_B(b_i)$, and the joint probability of the measurement of a and b is $P_{AB}(a_i, b_k)$. The mutual information I of two measurements a_i and b_k is symmetric and non-negative, and equals to zero if only the systems are independent. The average mutual information between any value a_i from system A and b_k from B is the average over all possible measurements of $I_{AB}(a_i, b_k)$,

$$I_{AB}(a_i, b_k) = \log_2\left(\frac{P_{AB}(a_i, b_k)}{P_A(a_i)P_B(b_k)}\right) \quad (4)$$

To place this definition to a context of observations from a certain physical system, let us think of the sets of measurements s(n) as the A and of the measurements a time lag τ later, $s(n + \tau)$, as

B set. The average mutual information between observations at n and n + τ is then

$$I_{AB}(\tau) = \sum_{a_i, b_k} P_{AB}(a_i, b_k) I_{AB}(a_i, b_k) \quad (5)$$

Now we have to decide what property of I(τ) we should select, in order to establish which among the various values of τ we should use in making the data vectors y(n). One could remind that the autocorrelation function and average mutual information can be considered as analogues of the linear redundancy and general redundancy, respectively, which was applied in the test for nonlinearity. The general redundancies detect all dependences in the time series, while the linear redundancies are sensitive only to linear structures. Further, a possible nonlinear nature of process resulting in the vibrations amplitude level variations can be concluded.

The goal of the embedding dimension determination is to reconstruct a Euclidean space R^d large enough so that the set of points d_A can be unfolded without ambiguity. In accordance with the embedding theorem, the embedding dimension, d_E, must be greater, or at least equal, than a dimension of attractor, d_A, i.e. $d_E > d_A$. However, two problems arise with working in dimensions larger than really required by the data and time-delay embedding [1-20]. First, many of computations for extracting interesting properties from the data require searches and other operations in R^d whose computational cost rises exponentially with d. Second, but more significant from the physical point of view, in the presence of noise or other high dimensional contamination of the observations, the extra dimensions are not populated by dynamics, already captured by a smaller dimension, but entirely by the contaminating signal. In too large an embedding space one is unnecessarily spending time working around aspects of a bad representation of the observations which are solely filled with noise. It is therefore necessary to determine the dimension d_A. There are several standard approaches to reconstruct the attractor dimension (see, e.g., [1-9]), but let us consider in this study two methods only. The correlation integral analysis is one of the widely used techniques to investigate the signatures of chaos in a time series. The analysis uses the correlation integral, C(r), to distinguish between chaotic and stochastic systems. To compute the correlation integral, the algorithm of Grassberger and Procaccia is the most commonly used approach. According to this algorithm, the correlation integral is

$$C(r) = \lim_{N\to\infty} \frac{2}{N(n-1)} \sum_{\substack{i,j \\ (1\le i<j\le N)}} H\left(r - |\, \mathbf{y}_i - \mathbf{y}_j \,|\right) \quad (6)$$

where H is the Heaviside step function with H(u) = 1 for u > 0 and H(u) = 0 for u ≤ 0, r is the radius of sphere centered on y_i or y_j, and N is the number of data measurements. If the time series is characterized by an attractor, then the integral C(r) is related to the radius r given by

$$d = \lim_{\substack{r\to 0 \\ N\to\infty}} \frac{\log C(r)}{\log r}, \quad (7)$$

where d is correlation exponent that can be determined as the slop of line in the coordinates log C(r) versus log r by a least-squares fit of a straight line over a certain range of r, called the scaling region.

If the correlation exponent attains saturation with an increase in the embedding dimension, then the system is generally considered to exhibit chaotic dynamics. The saturation value of the correlation exponent is defined as the correlation dimension (d_2) of the attractor. The method of surrogate data [1,8,9] is an approach that makes use of the substitute data generated in accordance to the probabilistic structure underlying the original data.

Often, a significant difference in the estimates of the correlation exponents, between the original and surrogate data sets, can be observed. In the case of the original data, a saturation of the correlation exponent is observed after a certain embedding dimension value (i.e., 6), whereas the correlation exponents computed for the surrogate data sets continue increasing with the increasing embedding dimension. It is worth consider another method for determining d_E that comes from asking the basic question addressed in the embedding theorem: when has one eliminated false crossing of the orbit with itself which arose by

virtue of having projected the attractor into a too low dimensional space? By examining this question in dimension one, then dimension two, etc. until there are no incorrect or false neighbours remaining, one should be able to establish, from geometrical consideration alone, a value for the necessary embedding dimension. Advanced version is presented in Refs. [8,9].

The Lyapunov's exponents (LE) are the dynamical invariants of the nonlinear system. In a general case, the orbits of chaotic attractors are unpredictable, but there is the limited predictability of chaotic physical system, which is defined by the global and local LE. A negative exponent indicates a local average rate of contraction while a positive value indicates a local average rate of expansion. In the chaos theory, the spectrum of LE is considered a measure of the effect of perturbing the initial conditions of a dynamical system. In fact, if one manages to derive the whole spectrum of the LE, other invariants of the system, i.e. Kolmogorov entropy (KE) and attractor's dimension can be found. The inverse of the KE is equal to an average predictability. Estimate of dimension of the attractor is provided by the Kaplan and Yorke conjecture:

$$d_L = j + \frac{\sum_{\alpha=1}^{j} \lambda_\alpha}{|\lambda_{j+1}|}, \qquad (8)$$

where j is such that $\sum_{\alpha=1}^{j} \lambda_\alpha > 0$ and $\sum_{\alpha=1}^{j+1} \lambda_\alpha < 0$, and the LE λ_α are taken in descending order. There are a few approaches to computing the LE. One of them computes the whole spectrum and is based on the Jacobi matrix of system. In the case where only observations are given and the system function is unknown, the matrix has to be estimated from the data. In this case, all the suggested methods approximate the matrix by fitting a local map to a sufficient number of nearby points. To calculate the spectrum of the LE from the amplitude level data, one could determine the time delay τ and embed the data in the four-dimensional space. In this point it is very important to determine the Kaplan-Yorke dimension and compare it with the correlation dimension, defined by the Grassberger-Procaccia algorithm. The estimations of the KE and average predictability can further show a limit, up to which the amplitude level data can be on average predicted. Other details can be found in Refs. [5-20].

3. Data on chaotic elements in time series of the radon concentration and conclusion

The concentration of atmospheric radon ^{222}Rn was determined by measuring the activity of beta particles in atmospheric aerosol using radon monitors. Measurements of the radon concentrations at SMEAR II station (61 ° 51'N, 24 ° 17'E, 181 m above sea level; near the Hyytiälä, Southern Finland) was done by group of experts of the Finnish Meteorological Institute (FMI) and was actually integrated into the system long-term measurements (see details in Ref.[74] and [75-77] too). The continuous measurement was performed during 2000-2006 on the seventh heights (from 4.2 m to 127 m). Technologically for the detection of beta particles there are used the device with a pair of the Geiger-Müller counters, arranged in the lead corymbs. Registration of the beta particles was cumulatively carried in 10-minutes intervals. Effectiveness of a detection was 0.96% and 4.3% for beta radiation from ^{214}Pb and ^{214}Bi respectively. Estimate of the 1-σ statistical counting - ± 20% for stable concentrations of ^{222}Rn (1 Bq/m^3). The mean-daily values of atmospheric ^{222}Rn concentrations were in the range from <0.1 to 11 Bq/m^3. In fact, the lower limit of this range was limited by a hardware detection limit of the radon monitors. The corresponding data meet the log-normal distribution with a geometric mean of 2.5 Bq/m^3 (a standard geometric deviation of 1.7 Bq/m^3). The average geometric value for the daily average radon concentrations was amounted to 2.3 to 2.6 Bq× m^{-3} per year. In general during 2000-2006 as hourly, as daily values of a parameter, which corresponds to the radon concentration, were ranged from about 1 to 5 Bq/m^3. In Figure 1 there is presented the typical time dependent curve of the radon concentration , received on the base of measurements at SMEAR II station (61 ° 51'N, 24 ° 17'E, 181 m above sea level; near the Hyytiälä, Southern Finland) (see [74]).

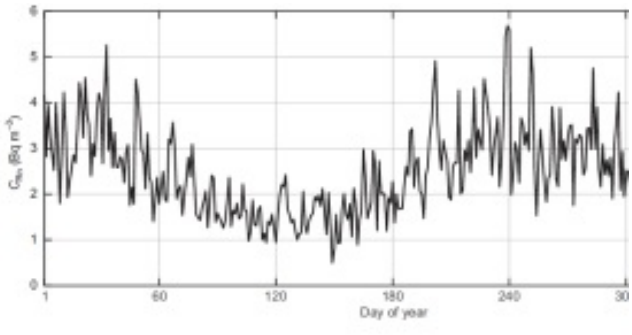


Figure 1. Time dependent curve of the radon concentration, received on the base of measurement (SMEAR II station)

Below in Table 1 we list the results of computing different dynamical and topological invriants and parameters (Time delay τ,correlation dimension (d_2), embedding space dimension (d_E), Lyapunov exponent (λ_i), Kolmogorov entropy (K_{ent}), Kaplan-York dimension (d_L), the predictability limit (Pr_{max}) and chaos indicator (K_{ch}) for radon concentration time series (2001).

Table 1. Time delay τ,correlation dimension (d_2), embedding space dimension (d_E), Lyapunov exponent (λ_i), Kolmogorov entropy (K_{ent}), Kaplan-York dimension (d_L), the predictability limit (Pr_{max}) and chaos indicator (K_{ch}) for the radon concentration time series (2001)

Year	τ	d_2	d_E
2001	12	5,48	6
Year	λ_1	λ_2	K_{ent}
2001	0,0182	0,0058	0,024
Year	d_L	Pr_{max}	K
2001	5,36	42	0,80

The resulting Kaplan- York dimension is very close to the correlation dimension, which is determined by the algorithm by Grassberger and Procaccia; Moreover, the Kaplan-York dimension is smaller than the dimension of attachment, which confirms the correctness of the choice of the latter. Therefore, using the new uniform chaos-dynamical approach we have carried out modeling and analysis of temporal evolution of the atmospheric radon ^{222}Rn concentration, firstly received data on topological and dynamical invariants for the time series of the ^{222}Rn concentration and discovered a deterministic chaos phenomenon. The results are of great theoretical and practical interest as for the dynamical systems and chaos theories for applied scientific applications such as nuclear physics, photoelectronics, atmospheric and environmental (environmental radioactivity) sciences etc.

References

1. Packard N.H., Crutchfield J.P., Farmer J.D., Shaw R.S., Geometry from a time series// Phys. Rev. Lett.–1990.–Vol.45.–P. 712–716.
2. Abarbanel H.D.I., Brown R., Sidorowich J.J., Tsimring L.Sh., The analysis of observed chaotic data in physical systems//Rev. Mod. Phys.–1993.–Vol.65.–P.1331–1392.
3. R. Gallager, Information theory and reliable communication (N.-Y.,Wiley, 1996).
4. Grassberger P, Procaccia I., Measuring the strangeness of strange attractors// Physica D. – 1993. – Vol. 9. – P. 189–208.
5. F. Takens in: Dynamical systems and turbulence, ed by D. Rand and L. Young (Springer, Berlin, 1991), pp.366–381; R. Mañé, in: Dynamical systems and turbulence, ed by D. Rand and L. Young (Springer, Berlin, 1991), pp.230–242.
6. 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.
7. A.V. Glushkov, Modern theory of a chaos, (Odessa, Astroprint, 2008), 450p.
8. G.P. Prepelitsa, Nonlinear dynamics of quantum and laser systems with ele-

ments of a chaos// Photoelectronics.-2014.-Vol.23.-P.96-106.
9. Glushkov A.V., Khetselius O.Y., Brusentseva S.V., Zaichko P.A., Ternovsky V.B., Studying interaction dynamics of chaotic systems within a non-linear prediction method: application to neurophysiology// Advances in Neural Networks, Fuzzy Systems and Artificial Intelligence, Series: Recent Advances in Computer Engineering, Ed. J.Balicki.-2014.-Vol.21.-P.69-75.
10. Glushkov A.V., Svinarenko A.A., Buyadzhi V.V., Zaichko P., Ternovsky V., Chaos-geometric attractor and quantum neural networks approach to simulation chaotic evolutionary dynamics during perception process// Advances in Neural Networks, Fuzzy Systems and Artificial Intelligence, Series: Recent Advances in Computer Engineering, Ed. J.Balicki.-2014.-Vol.21.-P.143-150.
11. 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.
12. Glushkov A.V., Khetselius O.Yu., Kuzakon V., Prepelitsa G.P., Solyanikova E.P., Svinarenko A., Modeling of interaction of the non-linear vibrational systems on the basis of temporal series analyses (application to semiconductor quantum generators)// Dynamical Systems-Theory and Applications.-2011.-BIF110.
13. Serbov N.G., Glushkov A.V., Bunyakova Yu.Ya., Prepelitsa G.P., Svinarenko A.A., Sensing the kinetical features of energy exchange in mixture CO_2-N_2-H_20 of atmospheric gases under interacting with laser radiation// Sensor Electr. and Microsyst. Techn.-2006.-N4.-P.20-22.
14. Glushkov A.V., Khetselius O.Y., Bunyakova Yu.Ya., Prepelitsa G.P., Solyanikova E.P., Serga E., Non-linear prediction method in short-range forecast of atmospheric pollutants: low-dimensional chaos// Dynamical Systems - Theory and Applications (Lodz).-2011.-P.39-44 (LIF111).
15. Glushkov A.V., Khetselius O.Yu., Prepelitsa G., 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 International Geometry Center».-2013.-Vol.6, N1.-P.43-48.
16. Khetselius O.Yu., Forecasting evolutionary dynamics of chaotic systems using advanced non-linear prediction method// Dynamical Systems – Theory and Applications, Eds. J. Awrejcewicz, M. Kazmierczak, P. Olejnik, J, Mrozowski.-2013.-Vol.1.-P.145-152.
17. Glushkov A.V., Kuzakon V.M., Ternovsky V.B., Buyadzhi V.V., Dynamics of laser systems with absorbing cell and backward-wave tubes with elements of a chaos// Dynamical Systems – Theory and Applications, Eds. J. Awrejcewicz, M. Kazmierczak, P. Olejnik, J, Mrozowski.-2013.-Vol. T1.-P.461-466.
18. Bunyakova Yu.Ya., Khetselius O.Yu., Non-linear prediction statistical method in forecast of atmospheric pollutants// Proc. of 8th International Carbon Dioxide Conference.-2009.-P.T2-098.
19. Glushkov A.V., Bunyakova Yu.Ya., Zaichko P., Geometry of Chaos: Consistent combined approach to treating chaotic dynamics atmospheric pollutants and its forecasting// Proc. International Geometry Center".-2013.-Vol.6, N3.-P.6-14.
20. 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.
21. 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.
22. 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.
23. Glushkov A.V., Khetselius O., Svinarenko A.A., Lovett L., Energy approach to nuclei and atoms in a strong laser field: Stark effect and multiphoton resonances // Quantum Theory: Reconsideration of Foundations. AIP Conference Proceedings.-2010.-Vol.1232.-P.228-234.
24. 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 Conference Proceedings.-2010.-Vol.1232.-P.259-266.
25. 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.
26. 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.
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., 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.
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., 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. Quant. Chem.-2009.-Vol.109,N14.-P.3473-3481.
31. 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.
32. 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.
33. 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.

34. 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.Brändas, G.Delgado-Barrio (Springer).-2015-Vol.29.-P.55-76.
35. 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.
36. 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.
37. 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.
38. 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.
39. Ternovsky V.B., Glushkov A.V., Zaichko P., 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.
40. 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.
41. 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.
42. Glushkov A.V., Relativistic and correlation effects in spectra of atomic systems.-Odessa: Astroprint.-2006.-400P.
43. Glushkov A.V., Atom in electromagnetic field.-Kiev: KNT, 2005.-450P.
44. 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.-523-540.
45. Glushkov A.V., Khetselius O., Svinarenko 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.
46. 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.
47. 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.
48. Malinovskaya S.V., Glushkov A.V., Khetselius O.Yu., Lopatkin Yu., Loboda A.V., Svinarenko 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,N2.-P.288-296.
49. Malinovskaya S.V., Glushkov A.V., Khetselius O.Yu., Svinarenko A.A., Mischenko E.V., Florko T.A., Optimized 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.
50. Glushkov A.V., Khetselius O.Y., Malinovskaya S.V., Spectroscopy of cooperative laser-electron nuclear effects in multiatomic molecules// Molec. Phys. (UK).-2008.-Vol.106.-N9-10.-P.1257-1260.
51. 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.541-558.
52. Glushkov A.V, Malinovskaya S.,Cooperative 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.
53. Khetselius O.Yu., Hyperfine structure of atomic spectra.-Odessa: Astroprint, 2008.-210P.
54. Khetselius O.Yu., Hyperfine structure of radium// Photoelectronics.-2005.-N14.-P.83-85.
55. Khetselius O., Spectroscopy of cooperative electron-gamma-nuclear processes in heavy atoms: NEET effect// J. Phys.: Conf. Ser.-2012.- Vol.397.-P.012012
56. 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.
57. 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.
58. 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.
59. 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.
60. Khetselius O.Yu., Quantum Geometry: New approach to quantization of the quasistationary states of Dirac equation for super heavy ion and calculating hyper fine structure parameters// Proc. Int. Geometry Center.-2012.-Vol.5,№ 3-4.-P.39-45.

61. 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.
62. 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.
63. 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.
64. 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.
65. Khetselius O.Yu., Hyperfine structure of energy levels for isotopes 73Ge, 75As, 201Hg// Photoelectronics.-2007.-N16.-P.129-132.
66. 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.
67. 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.
68. 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.
69. 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.
70. 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.
71. 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.
72. Buyadzhi V.V., Zaichko P.A., Gurskaya M., Kuznetsova A.A., Ponomarenko E.L., Ternovsky E.,Relativistic theory of excitation and ionization of Rydberg atoms in a Black-body radiation field//J. Phys.: Conf. Series.-2017.-Vol.810.-P. 012047.
73. 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.161-178.
74. Xuemeng Chen, Jussi Paatero, Veli-Matti Kerminen, Laura Riuttanen, etal Responses of the atmospheric concentration of radon-222 to the vertical mixing and spatial transportation// Boreal Environment Research (Helsinki) -2016 -Vol.21- P. 299–318.
75. Jacob D.J., Prather M.J. Radon-222 as a test of convective transport in a general circulation model// Tellus-1990-Vol.42b-P.118-134.
76. Jean-Louis Pinault, Jean-Claude Baubron Signal processing of diurnal and semidiurnal variations in radon and atmospheric pressure' A new tool for

accurate in situ measurement of soil gas velocity, pressure gradient, and tortuosity //Journal of Geophysical Research-1997-Vol. 102- N b8- P.18,101-18,120.
77. 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.

This article has been received within. April 2017.

UDC 541.13

O. Yu. Khetselius, A. V. Glushkov, V. V. Buyadzhi, Yu. Ya. Bunyakova

NEW NONLINEAR CHAOS-DYNAMICAL ANALYSIS OF ATMOSPHERIC RADON ^{222}Rn CONCENTRATION TIME SERIES FROM BETA PARTICLES ACTIVITY DATA OF RADON MONITORS

Summary

The work is devoted to the development of the theoretical foundations of new universal complex chaos-dynamical approach to analysis and prediction of the atmospheric radon ^{222}Rn concentration changing from beta particles activity data of radon monitors (with pair of the Geiger-Müller counters). The approach presented consistently includes a number of new or improved methods of analysis (correlation integral, fractal analysis, algorithms of average mutual information, false nearest neighbors, Lyapunov exponents, surrogate data, non-linear prediction schemes, spectral methods, etc.) to solve problems quantitatively complete modeling and analysis of temporal evolution of the atmospheric radon ^{222}Rn concentration . There are firstly received data on topological and dynamical invariants for the time series of the ^{222}Rn concentration, discovered a deterministic chaos phenomenon using detailed data of measurements of the radon concentrations at SMEAR II station of the Finnish Meteorological Institute.

Key words: chaotic dynamics, time series of the ^{222}Rn concentration, universal complex chaos-dynamical approach, analysis and prediction

УДК 541.13

О. Ю. Хецелиус, А. В. Глушков, В. В. Буяджи, Ю. Я. Бунякова

НЕЛИНЕЙНЫЙ ХАОС-ДИНАМИЧЕСКИЙ АНАЛИЗ ВРЕМЕННЫХ РЯДОВ КОНЦЕНТРАЦИЙ АТМОСФЕРНОГО РАДОНА ^{222}Rn НА ОСНОВЕ ДАННЫХ АКТИВНОСТИ БЕТА ЧАСТИЦ РАДОНОВЫХ МОНИТОРОВ

Резюме

Работа посвящена разработке теоретических основ нового универсального комплексного хаос-динамического подхода к анализу и прогнозированию временных изменений концентрации атмосферного радона ^{222}Rn на основе данных активности бета-частиц радоновых мониторов (с парой счетчиков Гейгера-Мюллера). Подход последовательно включает в себя ряд новых или улучшенных методов анализа (метод корреляционного интеграла, фрактальный анализ, алгоритмы средней взаимной информации, ложных ближайших соседей, показателей Ляпунова, схемы нелинейного прогнозирования, спектральные методы и т.д.) для решения проблемы количественно полного моделирования и анализа временной эволюции концентрации атмосферной радона ^{222}Rn. Впервые получены данные о топологических и динамических инвариантах для временных рядов концентрации ^{222}Rn, открыт феномен детерминированного хаоса, используя подробные данные измерений концентраций радона на станции SMEAR II Финского метеорологического института

Ключевые слова: Хаотическая динамика, временные ряды концентрации ^{222}Rn, универсальный комплексный хаос-динамический подход, анализ и прогнозирование

УДК 541.13

О. Ю. Хецеліус, О. В. Глушков, В. В. Буяджі, Ю. Я. Бунякова

НЕЛІНІЙНИЙ ХАОС-ДИНАМІЧНИЙ АНАЛІЗ ЧАСОВИХ СЕРІЙ КОНЦЕНТРАЦІЙ АТМОСФЕРНОГО РАДОНУ ^{222}Rn НА ОСНОВІ ДАНИХ АКТИВНОСТІ БЕТА ЧАСТИНОК РАДОНОВИХ МОНІТОРІВ

Резюме

Робота присвячена розробці теоретичних основ нового універсального комплексного хаос-динамічного підходу до аналізу та прогнозування часових змін концентрації атмосферного радону ^{222}Rn на основі даних активності бета-частинок радонових моніторів (з парою лічильників Гейгера-Мюллера). Підхід послідовно включає в себе ряд нових або поліпшених методів аналізу (метод кореляційного інтегралу, фрактальний аналіз, алгоритми середньої взаємної інформації, помилкових найближчих сусідів, показників Ляпунова, схеми нелінійного прогнозування, спектральні методи і т.і.) для вирішення проблеми кількісно повного моделювання та аналізу часової еволюції концентрації атмосферної радону ^{222}Rn. Вперше отримані дані про топологічні і динамічні інваріанти для часових рядів концентрації ^{222}Rn, відкрито феномен детермінованого хаосу, використовуючи детальні дані вимірювань концентрацій радону на SMEAR II станції Фінського метеорологічного інституту.

Ключові слова: Хаотична динаміка, часові ряди концентрації ^{222}Rn, універсальний комплексний хаос-динамічний підхід, аналіз і прогнозування

UDC 621.315.592

Yu. A. Nitsuk, Yu. F. Vaksman, I. V. Tepliakova, A. A. Rimashevskiy

I. I. Mechnikov Odesa National University
e-mail: nitsuk@onu.edu.ua

SYNTHESIS AND LUMINESCENCE PROPERTIES OF ZnSe:Al NANOPARTICLES

Colloidal nanocrystals of ZnSe:Al were synthesized in organic polymer matrices. The optical absorption and long-wavelength luminescence were studied, the average sizes of nanoparticles were determined, the efficiency of the transition from bulk crystals to nanocrystals was shown, and the types of optical transitions were determined.

Introduction

Semiconductor colloidal nanocrystals of the A_2B_6 group are promising materials for biomedical marking and visualization. The most widely represented in the studies are CdS and CdSe nanocrystals [1,2], which have tunable, wide and intense emission bands. However, many results show that any leakage of cadmium from nanocrystals will be toxic and fatal to biological systems. In connection with this, the synthesis of nanomaterials, not cadmium entities, is topical. Such materials include zinc chalcogenides, and zinc selenide in particular.

Being a wide-band semiconductor, ZnSe is ideally suited for the creation on its basis of optoelectronics devices and biomedical imaging. Doping ZnSe allows the realization of luminescent radiation in the visible and near infrared wavelengths. At present, ZnSe nanocrystals doped with transition elements such as Cu, Mn, Co have been successfully synthesized [3] At the same time, there is no information on the preparation of zinc selenide nanoparticles doped with Group III donor elements (Al, Ga, In). Investigations of the photoluminescence of bulk ZnSe: Al crystals showed that in zinc selenide an Al impurity is the best activator in the visible range [4]. So the preparation and investigation of the luminescent properties of ZnSe: Al nanocrystals is relevant.

The purpose of this work is the development of an ecological approach to the synthesis of ZnSe:Al nanocrystals, the study of their luminescent properties and the establishment of natural emission transitions in these nanocrystals.

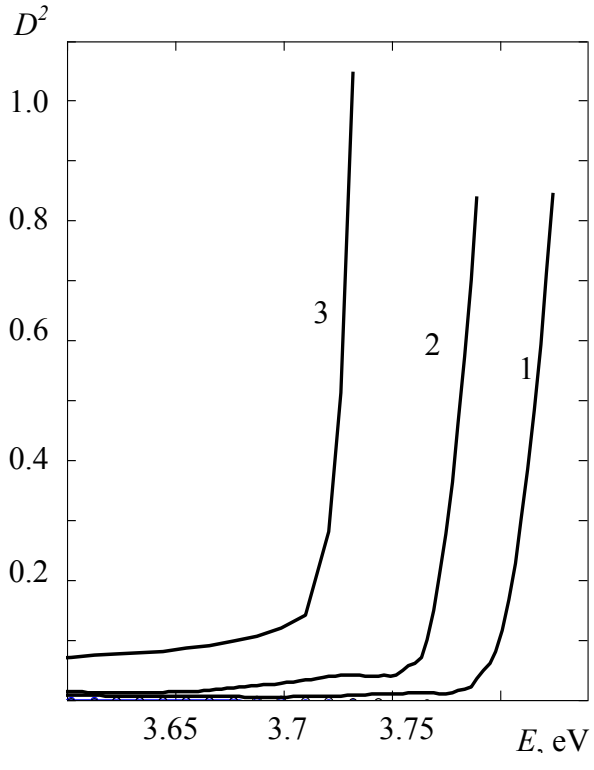
Experimental

The study used commercial reagents Beijing Reagent Company. $ZnCl_2$ was the source of zinc ions. The source of Se^{2-} ions was sodium selenosulfate Na_2SeSO_3, which was prepared with an aqueous Na_2SO_3 solution and powdered Se (99%). Polyvinyl alcohol, gelatin or lactose was used as the growth stabilizer of nanoparticles. The doping with Al ions was carried out by the addition of Al_2Cl_3. The resulting colloidal solution containing ZnSe and ZnSe:Al nanoparticles was deposited on quartz substrates, then the solvent evaporated, forming membranes for measuring optical absorption and photoluminescence.

The optical absorption and photoluminescence spectra were recorded with an MDR-6 monochromator with a 2400 grove$\cdot$ mm^{-1} diffraction gratings in the ultraviolet and 1200 grove$\cdot$ mm^{-1} in the visible range.

Investigation of the optical absorption

The optical density spectra of ZnSe and ZnSe:Al nanocrystals were studied. It is established that in all the samples studied the absorption edge is shifted to the region of high energies in comparison with the absorption edge of single crystals of ZnSe, which indicates the presence of quantum size effects in the samples. The influence of the ratio of the concentrations of zinc and selenium sources on the position of the absorption edge was established. The maximum displacement was observed at a ratio of $ZnCl_2$ to Na_2SeSO_3 of 10:1.



The mean radius of the ZnSe, ZnSe:Al particles was estimated from the change in the band gap (ΔE_g) relative to the bulk crystal, using the effective-mass approximation using the equation [5]

$$R = \frac{h}{\sqrt{8\ \Delta E_g}}. \qquad (1)$$

There h is the Planck constant; $\mu = ((m_{e^*})^{-1} + (m_{h^*})^{-1})^{-1}$, where $m_e^* = 0.17m_e$, $m_h^* = 0.6m_e$ are, respectively, the effective masses of the electron and hole in zinc selenide, m_e is the mass of the free electron; ΔE_g is the difference between the width of the band gap in the nanoparticle and the bulk crystal of ZnSe (2.68 eV). The results of calculations showed that the minimum ZnSe nanoparticles size (3.5 nm) is reached just at the ratio of $ZnCl_2$ to Na_2SeSO_3 10: 1 (Fig. 1, curve 1).

Doping of ZnSe nanocrystals with aluminum leads to a shift in the absorption edge to the region of lower energies. The magnitude of the displacement increased with increasing concentration of the aluminum source (Fig. 1, curves 2,3). A similar dependence of the width of the forbidden band on the concentration of the dopant was observed earlier in bulk ZnSe crystals containing the donor impurity In, the impurity ions of the transition elements, and was explained by the presence of an impurity Coulomb interaction [6]. Using relation

$$\Delta E_g = 2\cdot 10^5 \left(\frac{3}{\pi}\right)^{1/3} \frac{eN^{1/3}}{4\pi\varepsilon_0\varepsilon_s}, \qquad (2)$$

where: e – electron charge, N – concentration of impurities in cm^{-3}, $\varepsilon_s = 8.66$ is zinc selenide static dielectric constant, the concentration of aluminum impurity in the investigated nanocrystals is determined. 5% solution of Al_2Cl_3 corresponds to the concentration of aluminum in nanocrystals of 10^{18} cm^{-3}, and 10% solution of Al_2Cl_3 is a concentration of 10^{19} cm^{-3}.

Investigation of long-wavelength photoluminescence

Investigation of ZnSe nanocrystals photoluminescence spectra is showed the presence of broad photoluminescence bands localized in the 550-850 nm region. The change in the temperature of nanocrystals from 300 to 430 K did not cause a shift in the spectra studied. The position of the spectra remained unchanged even with a change in the width of the forbidden band of nanocrystals. The presence of a number of bend and a large (~ 150 nm) half-width of the bands indicate their non-elementary nature. The decomposition into elementary Gaussian components in the Origin-Pro 7 program revealed a series of elementary emission lines localized at 580, 600, 630, 680, 700, 750 and 800 nm (Fig. 2, a). The identical elementary emission lines were observed earlier in bulk ZnSe single crystals (Fig. 2, b) [4].

Emission at a wavelength of 580 nm appears due to associative native defects $(V_{Zn}V_{Se})^-$. The emission line at a wavelength of 600 nm appears due to associative defects $(V_{Zn}D_{Se})^-$ where the donor is either V_{Se} or an uncontrolled donor impurity, an IIV group element, for example, Cl, Br, I. The other emission lines were associated with defects $(V_{Zn}D_{Zn})^-$ with different distances between donors and acceptors. Here the donor, according to [4], is the uncontrolled impurities Al, In, Ga.

Doping with aluminum during the growth of nanocrystals leads to an increase in the emission intensity in the 500-1000 nm region. Further increase of the emission intensity with increasing

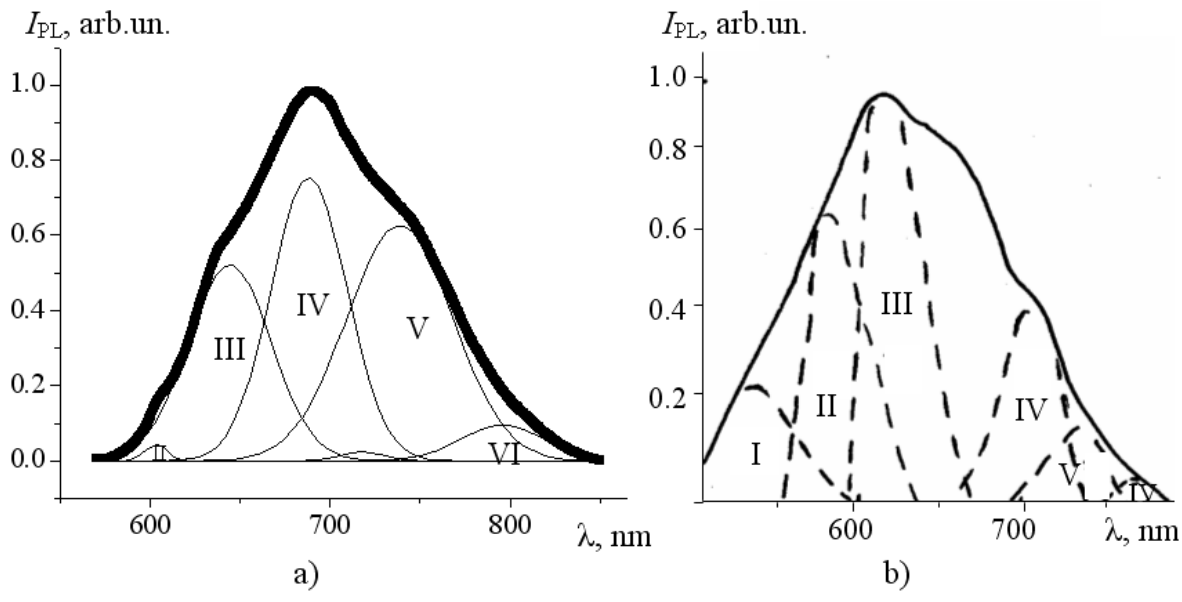


Fig 2. Photoluminescence spectra of (1) ZnSe nanocrystals and (b) ZnSe bulk crystals [4].

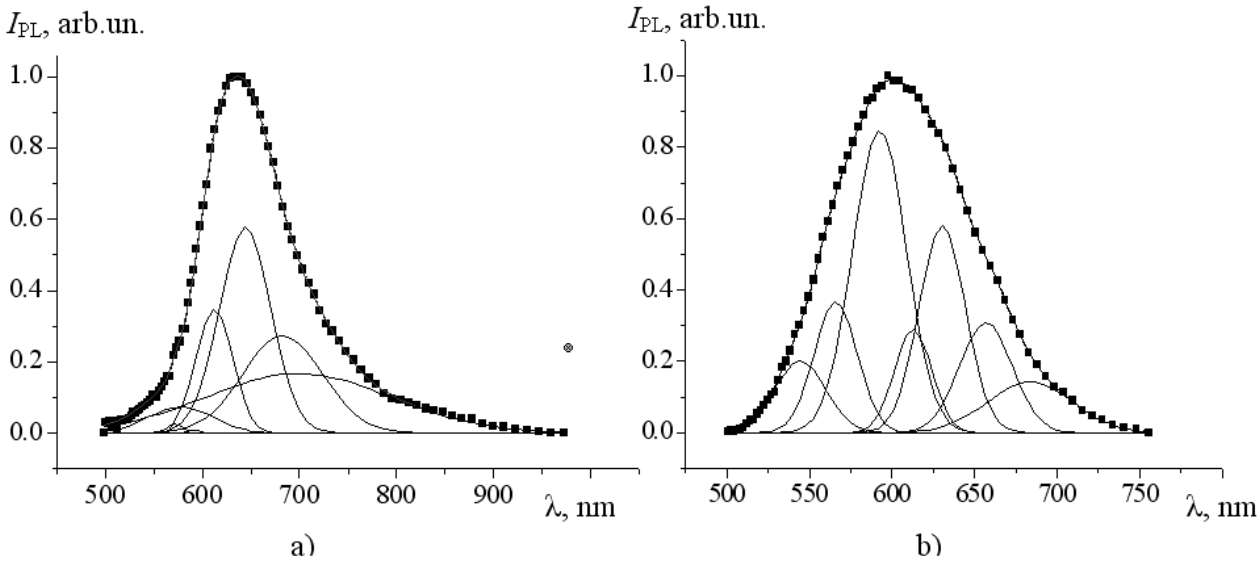


Fig 3. Photoluminescence spectra of (a) ZnSe:Al nanocrystals and (b) ZnSe:Al bulk crystals.

Al_2Cl_3 concentration is explained by an increase of the donor impurity concentration in investigated nanocrystals.

In the emission spectra of ZnSe:Al nanocrystals, elementary emission lines are emitted at 580, 600, 630, 680, and 700 nm. The same emission lines were detected in bulk crystals of ZnSe:Al (Fig. 3, b).

It is established that a change of Al_2Cl_3 concentration, the choice of the stabilizing matrix type does not lead to a shift of the elementary and integral emission lines to the short-wave or long-wave region. The change in technological conditions leads to a change in the intensity of the elementary emission lines, which is explained by the redistribution of the concentration of native and impurity defects that make up the associative centers. The shift of the emission integrated maximum to the smaller wavelengths region with increasing Al_2Cl_3 concentration from 2 to 10% can be explained by increasing in the intensity of the elementary emission line at 600 nm due to associative defects $(V_{Zn}Cl_{Se})^-$.

Conclusions

ZnSe and ZnSe: Al nanoparticles up to 3.5 nm in diameter were successfully synthesized using the "green" synthesis method and organic stabilizing agents. It is shown that ZnSe:Al nanoparticles possess effective long-wave emission and can be used as fluorescent labels. The nature of the radiative transitions in ZnSe and ZnSe:Al nanocrystals is established. It has been experimentally confirmed that when the transition from bulk crystals to nanocrystals does not occur, the emission lines shift toward donor-acceptor pairs.

References

1. X. Peng, M. C. Schlamp, A. V. Kadavanich, and A. P. Alivisatos, "Epitaxial growth of highly luminescent CdSe/CdS core/shell nanocrystals with photostability and electronic accessibility," Journal of the American Chemical Society, vol. 119, no. 30, pp. 7019-7029, 1997.
2. B. O. Dabbousi, J. Rodriguez-Viejo, F. V. Mikulec et al., "(CdSe)ZnS core-shell quantum dots: synthesis and characterization of a size series of highly luminescent nanocrystallites," Journal of Physical Chemistry B, vol. 101, no. 46, pp. 9463– 9475, 1997.
3. D Han, C. Song X. Li. Synthesis and Fluorescence Property of Mn-Doped ZnSe Nanowires // J. Nanomaterials. – 2010. - P.1-4.
4. Serdyuk V.V., Korneva N.N., Vaksman Yu.F. Studies of Long-Wave Luminescence of Zinc Selenide Monocrystals // Phys. Stat. Sol.(a). – 1905. – V.91. – P. 173-183.
5. Гусев А.И., Рempель А.А. Нанокристаллические материалы. – М:Физматлит. – 2000. –С 224.
6. Vaksman Yu.F., Nitsuk Yu.A., Purtov Yu.N. and Shapkin P.V. Native and Impurity Defects in ZnSe:In Single Crystals Prepared by Free Growth// Semiconductors. – 2001. – V. 35, № 8. – P. 920-926.

This article has been received in May 2017

UDC 621.315.592

Yu. A. Nitsuk, Yu. F. Vaksman, I. V. Tepliakova, A. A. Rimashevskiy

SYNTHESIS AND LUMINESCENCE PROPERTIES OF ZnSe:Al NANOPARTICLES

Summary

Colloidal nanocrystals of ZnSe:Al were synthesized in organic polymer matrices. The optical absorption and long-wavelength luminescence were studied, the average sizes of nanoparticles were determined, the efficiency of the transition from bulk crystals to nanocrystals was shown, and the types of optical transitions were determined.

Key words: ZnSe, ZnSe:Al, nanoparticles, colloidal synthesis, optical properties, luminescence, biomedical markers.

УДК 621.315.592

Ю. А. Ніцук, Ю. Ф. Ваксман, І. В. Теплякова, О. А. Рімашевський

СИНТЕЗ ТА ЛЮМІНЕСЦЕНТНІ ВЛАСТИВОСТІ НАНОКРИСТАЛІВ ZnSe:Al

Анотація

Колоїдні наночастинки ZnSe:Al були синтезовані в органічній полімерній матриці. Були досліджені оптичне поглинання та довгохвильова фотолюмінесценція. За зсувом ширини забороненої зони визначений середній розмір наночастинок. Визначена природа випромінювальних переходів.

Ключові слова: ZnSe, ZnSe:Al, наночастинки, колоїдний синтез, оптичні властивості, люмінесценція, біомаркери.

УДК 621.315.592

Ю. А. Ницук, Ю. Ф. Ваксман, И. В. Теплякова, А. А. Римашевский

СИНТЕЗ И ЛЮМИНЕСЦЕНТНЫЕ СВОЙСТВА НАНОКРИСТАЛЛОВ ZnSe:Al

Аннотация

Коллоидные наночастицы ZnSe:Al были синтезированы в органичеbской полимерной матрице. Были исследованы оптическое поглощение идлинноволновая люминесценция. По смещению ширины запрещенной зоны определялся средний раз мер наночастиц. Определена природа излучательных переходов.

Ключевые слова: ZnSe, ZnSe:Al, наночастицы, коллоидный синтез, оптические свойства, люминесценция, биомаркеры.

UDC 539.184

V. F. Mansarliysky, E. V. Ternovsky, A. V. Ignatenko, E. L. Ponomarenko

Odessa State Environmental University, 15, Lvovskaya str., Odessa, Ukraine
e-mail: ignatenkoav13@gmail.com

OPTIMIZED RELATIVISTIC DIRAC-FOCK APPROACH TO CALCULATING THE HYPERFINE LINE SHIFT AND BROADENING FOR HEAVY ATOMS IN THE BUFFER GAS

It is presented a new consistent relativistic approach to description of the energetic and spectral properties of the heavy atoms in an atmosphere of the inert gases, based on the atomic gauge-invariant relativistic perturbation theory with the optimized Dirac-Fock zeroth approximation with density functional correlation potential and the exchange perturbation theory for construction of the interatomic potential function. As illustration it is applied to calculating the interatomic potentials, hyperfine structure line collision shift and broadening for alkali and thallium atoms, in an atmosphere of the buffer inert gas. It is shown that an accurate accounting of relativistic and exchange-correlation provides physically reasonable description of the energetic and spectral properties of the heavy atoms in an atmosphere of the inert gases.

1. Introduction

In Ref. [1-3] It has been presented a new consistent relativistic approach to hyperfine structure line collision shift and broadening for heavy atoms in an atmosphere of the buffer inert gas, based on the atomic gauge-invariant relativistic perturbation theory and the optimal construction of the interatomic potential function within exchange perturbation theory . As illustration it has been applied to calculating the interatomic potentials, hyperfine structure line collision shift for heavy atoms, namely, rubidium, cesium etc in an atmosphere of the buffer inert gas (He). It was shown that the consistent, accurate accounting the the relativistic and exchange-correlation, continuum pressure effects has to be done to get an adequate description of the energetic and spectral properties of the heavy atoms in an atmosphere of the heavy inert gases.

Let us remind that the broadening and shift of atomic spectral lines by collisions with neutral atoms has been studied extensively since the very beginning of atomic physics, physics of collisions etc [4–36]. These studied are of a great interest for modern atomic and molecular spectroscopy, quantum chemistry, laser physics and quantum electronics, astrophysics and metrology as well as for studying a role of weak interactions in atomic optics and heavy-elements chemistry [37-48]. It is very important point that the computing the hyperfine structure line shift and broadening allows to check a quality of the orbitals basis and understand physical aspects of accounting the relativistic and correlation effects to the energetic and spectral characteristics of the two-center (multicenter) atomic systems. One of the known and widely used quantum methods to compute atomic parameters and spectral lines characteristics is the Dirac-Fock method. However, because of the known points connected with generation of non-optimized basis of wave functions and other ones (for example, the slow convergence of the corresponding PT series with the Dirac-Fock zeroth approximation, necessity of accurate accounting for the correlation effects etc) this method should be seriously improved. The most known improvement is in using the multiconfiguration Dirac-Fock approach.

In this paper we present a new consistent relativistic approach to description of the energetic and spectral properties of the heavy atoms in an atmosphere of the inert gases, based on the atomic gauge-invariant relativistic perturbation theory with the optimized Dirac-Fock zeroth approximation with density functional correlation potential and the exchange perturbation theory for construction of the interatomic potential function. As

illustration it is applied to calculating the, hyperfine structure line shift and broadening for alkali atoms in an atmosphere of the buffer inert gas. It is shown that an accurate accounting of relativistic and exchange-correlation provides physically reasonable description of the energetic and spectral properties of the heavy atoms in an atmosphere of the inert gases

2. Method

The basic expressions for the collision shift and broadening hyperfine structure spectral lines are taken from the kinetic theory of spectral lines [6,7,11,12]. In order to calculate a collision shift of the hyperfine structure spectral lines one can use the following expression known in the kinetic theory of spectral lines shape (see Refs. [1-7]):

$$f_p = \frac{D}{p} = \frac{4\pi w_0}{kT}\int_0^\infty [1+g(R)]dw(R)\exp\left(-U(R)/kT\right)R^2 dR \qquad (1)$$

$$g(R) = \begin{cases} \dfrac{2}{3\sqrt{\pi}}\left(-\dfrac{U(R)}{kT}\right)^{3/2}, & U<0, \\ 0, & U>0, \end{cases}$$

Here *U(R)* is an effective potential of interatomic interaction, which has the central symmetry in a case of the systems *A—B (*in our case, for example, *A*=Rb,Cs*; B*=He*)*; *T* is a temperature, w_0 is a frequency of the hyperfine structure transition in an isolated active atom; $d\omega(R)=Dw(R)/w_0$ is a relative local shift of the hyperfine structure line; $(1+g(R))$ is a temperature form-factor.

The local shift is caused due to the disposition of the active atoms (say, the alkali atom and helium He) at the distance *R*. In order to calculate an effective potential of the interatomic interaction further we use the exchange perturbation theory formalism (the modified version EL-HAV) [4-6]).

Since we are interested by the alkali (this atom can be treated as a one-quasiparticle systems, i.e. an atomic system with a single valence electron above a core of the closed shells) and the rare-earth atoms (here speech is about an one-, two- or even three-quasiparticle system), we use the classical model for their consideration. The interaction of alkali (A) atoms with a buffer (B) gas atom is treated in the adiabatic approximation and the approximation of the rigid cores. Here it is worth to remind very successful model potential simulations of the studied systems (see, for example, Refs. [13-26]).

In the hyperfine interaction Hamiltonian one should formally consider as a magnetic dipole interaction of moments of the electron and the nucleus of an active atom as an electric quadrupole interaction (however, let us remind that, as a rule, the moments of nuclei of the most (buffer) inert gas isotopes equal to zero).

The necessity of the strict treating relativistic effects causes using the following expression for a hyperfine interaction operator H_{HF} (see, eg., [3,5]):

$$H_{\mathrm{HF}} = a\sum_{i=1}^{N} I\frac{\alpha_i \times r_i}{r_i^3},\ a = -2\mu\frac{e^2 h}{2m_p c}\ , \qquad (2)$$

where I – the operator of the nuclear spin active atom, α_i – Dirac matrices, m_p – proton mass, μ - moment of the nucleus of the active atom, expressed in the nuclear Bohr magnetons. Of course, the summation in (2) is over all states of the electrons of the system, not belonging to the cores. The introduced model of consideration of the active atoms is important to describe an effective interatomic interaction potential (an active atom – an passive atom), which is centrally symmetric ($J_A=1/2$) in our case (the interaction of an alkali atom with an inert gas atom). Let us underline that such an approximation is also acceptable in the case system "thallium atom – an inert gas atom" and some rare-earth atoms, in spite of the presence of p-electrons in the thallium (in the case of rare-earth atoms, the situation is more complicated).One of the most correct methods to describe heavy atoms in an atmosphere of inert gases is the relativistic Dirac-Fock one or the Dirac-Kohn-Sham method. It is obvious that more sophisticated relativistic many-body methods should be used for correct treating relativistic, exchange-correlation and even nuclear effects in heavy atoms (including the many-body correlation effects, intershell correlations, possibly the continuum pressure etc]). In our calculation we

have used the relativistic functions, which are generated within the optimized Dirac-Fock zeroth approximation of the relativistic many body perturbation theory [38]. The potential of the inter-electron interaction with accounting the retarding effect and magnetic interaction in the lowest order on parameter α^2 (the fine structure constant) is as follows:

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

where ω_{ij} is the transition frequency; $\boldsymbol{\alpha}_i, \boldsymbol{\alpha}_j$ are the Dirac matrices. The PT zeroth approximation is the optimized Dirac-Fock one (plus additional correlation potential [15]) with using the consistent relativistic energy approach in order to construct the optimal relativistic orbitals basis (for details see Refs. [37-49]). The optimization is reduced to minimization of the gauge dependent multielectron contribution $Im\boldsymbol{\delta}E_{ninv}$ of the lowest relativistic perturbation theory corrections to the radiation widths of atomic levels. The minimization of the functional $Im\boldsymbol{\delta}E_{ninv}$ leads to the Dirac-Fock-like equations for the electron density that are numerically solved. The further elaboration of the method can be reached by means of using the Dirac-Sturm approach [5]. To calculate an effective potential of the interatomic interaction we use a method of the exchange perturbation theory (in the modified version EL-HAV [2,5,6]). Within exactness to second order terms on potential of Coulomb interaction of the valent electrons and atomic cores a local shift can be written as:

$$\delta\omega(R) = \frac{S_0}{1 - S_0} + \Omega_1 + \Omega_2 - \sum_n \frac{C_n}{R^n}, \qquad (4)$$

where values Ω_1, Ω_2 are the non-exchange and exchange non-perturbation sums of the first order correspondingly, which express through the matrix elements of the hyperfine interaction operator. The other details are in Refs.[1-11].

3. Results and conclusion

Further we present some test results of our studying hyperfine line collisional shift for alkali atoms (rubidium and caesium) in the atmosphere of the helium gas. In Table 1 and we present our theoretical results for the hyperfine line observed shift f_p (1/Torr) in a case of the Cs-He pairs. The experimental and alternative theoretical results by Batygin et al [5] for f_p are listed too. At present time there are no precise experimental data for a wide interval of temperatures in the literature. The theoretical data from Refs. [5] are obtained on the basis of calculation within the exchange perturbation theory with using the He wave functions in the Clementi-Rothaane approximation (column: Theory[a]), and in the Z-approximation (column: Theory[b]), and in the Löwdin approximation (column: Theory[c]).

Table 1

The observed f_ρ (10^{-9} 1/Torr) shifts for the systems of the Cs-He and corresponding theoretical data (see text)

T, K	Exp	a	b	c	This
223	-	164	142	169	173
323	135	126	109	129	134
423	-	111	96	114	121
523	-	100	85	103	109
623	-	94	78	96	102
723	-	-	-	-	95
823	-	-	-	-	90

Note:[a] –calculation with the He wave functions in the Clementi-Rothaane approximation; [b] – the Z-approximation; [c] –Löwdin approximation [5];

In Tables 2 there are listed the values of the observed f_ρ (10^{-9} 1/Torr) shifts for the systems of the pair: TI- He: C –our data, B- data by Mishchenko et al [7], A- data by Batygin-Sokolov [6]. In Table 3 there are listed the calculated adiabatic broadening values Γ_a/p (in Hz/Tor) for the thallium spectral lines for different temperatures and pairs TI-He, Kr, Xe.

Table 2

The observed f_ρ (10^{-9} 1/Torr) shifts for the systems of the pair: TI- He: C –our data, B- data by Mischenko et al [7], A- data by Batygin-Sokolov [6].

T, K	A	B	C
700	155	137	133,1
800	151	134	130,2
900	147.5	131	128,0
1000	143	126	123,4

Note: Exp. Value (Tl-He, T=700K): 130±10;

Table 3

Adiabatic broadening values Γ_a/p (in Hz/Tor) for the thallium spectral lines for different temperatures (pair: TI- He, TI-Kr, TI-Xe).

T, K	TI-He [4]	TI-He Our	TI-Kr Our	TI- Xe Our
700	2.83	2.49	6.79	17.27
800	2.86	2.52	5.88	14.58
900	2.90	2.56	5.24	12.87
1000	2.89	2.53	5.22	11.48

Our data confirm violation of the known Foli relationship between the observed f_ρ shift and the adiabatic broadening value ($\Gamma_a/p \sim f_\rho$) in the standard theory of spectral lines, for spectral. One culd see, that for example, $(\Gamma_a/p)/ f_p \sim 1/60$ for system of TI-He etc. Qualitatively similar , but quantitatively a little other estimates have been obtained in Refs. [3,4].

To conclude, let us underline that using the optimized relativistic orbitals basis (in our approach speech is about the optimized Dirac-Fock zeroth approzimation with additional correlation potential) and consistent precise accounting for the exchange-correlation and other effects is principally necessary for the physically reasonable description of the energetic and spectral properties of the heavy atoms in an atmosphere of the inert gases.

References

1. Mansarliysky V.F., New relativistic approach to calculating the hyperfine line shift and broadening for heavy atoms in the buffer gas //Photoelectronics.-2016.-Vol.25.-P.73-78.
2. Svinarenko A.A., Glushkov A.V. , Mansarliysky V.F., Mischenko E.V. Relativistic theory of shift and broadening spectral lines of the hyperfine transitions for heavy atoms in atmosphere of buffer inert gases/ -Odessa: OSENU.-2008.-120P.
3. Glushkov A.V.,Mansarliysky V.F., Khetselius O.Yu., Ignatenko A.V., Smirnov A.V., Prepelitsa G.P., Collisional shift of hyperfine line for thallium in an atmosphere of the buffer inert gas// J. of Physics: C Series (IOP).-2017.-Vol.810.-P. 012034.
4. 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.Brändas, G. Delgado-Barrio (Springer).-2015-Vol.29.-P.55-76.
5. Batygin V.V., Gorny M.B., Gurevich B.M., The interatomic potentials shifts lines HF structure and diffusion coefficients of rubidium and cesium atoms in a helium buffer//J. Tech.Fiz.-1998-Vol.48.-P.1097-1105.
6. Batygin V. V., Sokolov I. M., Collisional shift and adiabatic broadening of line of the hyperfine transition in the ground state of thallium in an atmosphere of buffer helium, krypton, xenon//Opt. Spectr.-1993.-Vol.55.-P.30-38.
7. Mischenko E., Loboda A., Svinarenko A., Dubrovskaya Yu.V., Quantum measure of frequency and sensing colli-

sional shift of the ytterbium hyperfine lines in medium of helium gas// Sensor Electr. and Microsyst. Techn.-2009.-N1.-P.25-29.
8. 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 atmosphere of inert gas// Phys.Scripta (IOP).-2013.-Vol.T153-P. 014037.
9. Glushkov A.V., Khetselius O.Yu., Lopatkin Yu.M., Florko T.A., Kovalenko O.A., Mansarliysky V.F., Collisional shift of hyperfine line for rubidium in an atmosphere of the buffer inert gas// Journal of Physics: C Series (IOP).-2014.-Vol.548.-P. 012026.
10. Khetselius O.Yu., Hyperfine structure of atomic spectra.- Odessa: Astroprint, 2008.
11. Khetselius O.Yu., Hyperfine structure of radium// Photoelectronics.-2005.-N14.-P.83-85.
12. Khetselius O., Spectroscopy of cooperative electron-gamma-nuclear processes in heavy atoms: NEET effect// J. Phys.: Conf. Ser.-2012.- Vol.397.-P.012012
13. 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. Techn. Phys.-1997.-Vol.38, Iss.2.-P.215-218
14. 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.
15. 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.
16. 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.
17. Glushkov A.V., Khetselius O.Y., Brusentseva S.V., Zaichko P.A., Ternovsky V.B., Studying interaction dynamics of chaotic systems within a non-linear prediction method: application to neurophysiology// Advances in Neural Networks, Fuzzy Systems and Artificial Intelligence, Ser: Recent Adv. in Computer Engineering,J.Balicki.-2014.-Vol.21-P.69-75
18. Khetselius O.Yu., Quantum Geometry: New approach to quantization of the quasistationary states of Dirac equation for super heavy ion and calculating hyper fine structure parameters// Proc. Int. Geometry Center.-2012.-Vol.5,№ 3-4.-P.39-45.
19. 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.
20. 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.
21. Khetselius O.Yu., Relativistic calculating the spectral lines hyperfine structure parameters for heavy ions// Spectral Line Shapes, AIP Conf.Proc. - 2008.-Vol.1058.-P.363-365.
22. 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.
23. Khetselius O.Yu., Hyperfine structure of energy levels for isotopes 73Ge, 75As, 201Hg// Photoelectronics.-2007.-N16.-P.129-132.

24. 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.
25. 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.
26. 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.
27. 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.
28. Glushkov A.V., Khetselius O.Yu., Kuzakon V., Prepelitsa G.P., Solyanikova E.P., Svinarenko A., Modeling of interaction of the nonlinear vibrational systems on the basis of temporal series analyses (application to semiconductor quantum generators)// Dynamical Systems-Theory and Applications.-2011.-BIF110.
29. 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.-P.94-98.
30. 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 Conf. Proceedings.-2008.-Vol.1058.-P.175-177
31. 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.
32. Glushkov A.V., Energy approach to resonance states of compound super-heavy nucleus and EPPP in heavy nucleus collisions// Low Energy Antiproton Phys. AIP Conference Proceedings.-2005.-Vol.796.-P.206-210.
33. Malinovskaya S.V., S.V., Dubrovskaya Yu., Vitavetskaya L., Advanced quantum mechanical calculation of the beta decay probabilities//Low Energy Antiproton Phys. AIP Conf. Proceedings.-2005.-Vol.796.-P.201-205.
34. 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.
35. 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. Series: Frontiers in Theoretical Chemistry and Physics, Eds. P.Hoggan, E.Brandas,J.Maruani, G. Delgado-Barrio, P.Piecuch (Springer).-2012.-Vol.22.-P.51-68.
36. 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.-523 p.
37. 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 F. Duarte (InTech).-2010.-P.159-186.
38. Glushkov A.V., Atom in electromagnetic field.-Kiev: KNT, 2005.-450P.; Glushkov A.V., Relativistic and cor-

relation effects in spectra of atomic systems.-Odessa: Astroprint.-2006.-400P.
39. 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.
40. 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. Int. Geometry Center".-2013.-Vol.6, N1.-P.43-48.
41. 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.
42. Malinovskaya S.V., Glushkov A.V., Khetselius O.Yu., Lopatkin Yu., Loboda A.V., Svinarenko A., Nikola L., Perelygina T., Generalized energy approach to calculating electron collision cross-sections for multicharged ions in a plasma: Debye shielding model// Int. J. Quant. Chem.-2011.-Vol.111.-P.288-296.
43. Malinovskaya S.V., Glushkov A.V., Khetselius O.Yu., Svinarenko A.A., Mischenko E.V., Florko T., Optimized perturbation theory scheme for calculating the interatomic potentials and hyperfine lines shift for heavy atoms in the buffer inert gas//Int. J. Quant. Chem.-2009.-Vol.109,N14.-P.3325-3329.
44. Glushkov A.V., Khetselius O.Y., Malinovskaya S.V., Spectroscopy of cooperative laser-electron nuclear effects in multiatomic molecules// Molec. Phys. (UK).-2008.-Vol. 106.-N9-10.-P.1257-1260.
45. 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.
46. Glushkov A.V, Malinovskaya S.,Cooperative 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 Sci.-2003.-P.242-250.
47. Glushkov A.V., Effective quasi-particle valence hamiltonian of molecules in the comprehensive semi-empirical theory// Sov. Journ. Struct. Chem.-1998.-Vol.29,N4.-P.3-9.
48. 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.
49. 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.

UDC 539.184

V. F. Mansarliysky, E. V. Ternovsky, A. V. Ignatenko, E. L. Ponomarenko

OPTIMIZED RELATIVISTIC DIRAC-FOCK APPROACH TO CALCULATING THE HYPERFINE LINE SHIFT AND BROADENING FOR HEAVY ATOMS IN THE BUFFER GAS

Summary

It is presented a new consistent relativistic approach to description of the energetic and spectral properties of the heavy atoms in an atmosphere of the inert gases, based on the atomic gauge-invariant relativistic perturbation theory with the optimized Dirac-Fock zeroth approximation with density functional correlation potential and the exchange perturbation theory for construction of the interatomic potential. As illustration it is applied to calculating the hyperfine structure line collision shift and broadening for alkali and thallium atoms in an atmosphere of the buffer inert gas. It is shown that an accurate accounting of relativistic and exchange-correlation provides physically reasonable description of the energetic and spectral properties of the heavy atoms in an atmosphere of the inert gases.

Keywords: Relativistic many-body perturbation theory, Dirac-Fock approximation, hyperfine line collision shift

УДК 539.184

В. Ф. Мансарлийский, Е. В. Терновский, А. В. Игнатенко, Е. Л. Пономаренко

НОВЫЙ РЕЛЯТИВИСТСКИЙ ПОДХОД К ОПРЕДЕЛЕНИЮ СДВИГА И УШИРЕНИЯ ЛИНИЙ СВЕРХТОНКОЙ СТРУКТУРЫ В ТЯЖЕЛЫХ АТОМАХ В БУФЕРНЫХ ГАЗАХ

Резюме

Представлен новый релятивистский подход к определению сдвига и уширения линии сверхтонкой структуры тяжелых атомов в атмосфере буферных газов, который базируется на атомной калибровочно-инвариантной релятивистской теории возмущений с оптимизированным нулевым приближением Дирака-Фока с дополнительным корреляционным потенциалом и обменной теории возмущений для построения межатомного потенциала. В качестве иллюстрации приведены результаты расчета сдвига и уширения сверхтонких линий ряда тяжелых атомов, в частности, щелочных и атома таллия, в атмосфере буферных инертных газов. Показано, что аккуратный учет релятивистских, обменно-корреляционных эффектов обеспечивает адекватное описание энергетических и спектральных свойств тяжелых атомов в атмосфере тяжелых инертных газов.

Ключевые слова: релятивистская теория возмущений, приближение Дирака-Фока, столкновительный сдвиг линий сверхтонкой структуры

УДК 539.184

В. Ф. Мансарлійський, Є. В. Терновський, Г. В. Ігнатенко, О. Л. Пономаренко

НОВИЙ РЕЛЯТИВІСТСЬКИЙ ПІДХІД ДО ВИЗНАЧЕННЯ ЗСУВУ ТА УШИРЕННЯ ЛІНІЙ НАДТОНКОЇ СТРУКТУРИ У ВАЖКИХ АТОМАХ В БУФЕРНИХ ГАЗАХ

Резюме

Представлений новий релятивістський підхід до визначення зсуву і уширення лінії надтонкої структури важких атомів в атмосфері буферних газів, який базується на атомній калібрувально-інваріантній релятивістській теорії збурень з оптимізованим нульовим наближенням Дірака-Фока з додатковим кореляційним потенціалом і обмінній теорії збурень для побудови міжатомного потенціалу. Як ілюстрація, наведені результати розрахунку зсуву і уширення надтонких ліній ряду важких атомів, зокрема, лужних і атома талію, в атмосфері буферних інертних газів. Показано, що акуратне урахування релятивістських, обмінно-кореляційних ефектів забезпечує адекватний опис енергетичних і спектральних властивостей важких атомів в атмосфері важких інертних газів.

Ключові слова: релятивістська теорія збурень, наближення Дірака-Фока, зсув за рахунок зіткнень ліній надтонкої структури

UDC 539.186

Yu. V. Dubrovskaya[1], A. A. Kuznetsova[2], A. S. Kvasikova[1], T. N. Sakun[3]

[1]Odessa State Environmental University, 15, Lvovskaya str., Odessa, 65016
[2]Odessa National Maritime Academy, Didrikhsona str. 4, Odessa, 65001
[3]National Aviation University, 1, Komarov Ave, 03680 Kiev, Ukraine
E-mail: dubrovskayayv@gmail.com

SPECTROSCOPY OF COOPERATIVE ELECTRON-γ- NUCLEAR EFFECTS IN MULTIATOMIC MOLECULES: MOLECULE XY_4

The consistent quantum approach to calculating the electron-nuclear γ transition spectra (a set of the vibration-rotational satellites in a molecule) of a nucleus in the multiatomic molecules is used to get the accurate spectroscopic data on the vibration-nuclear transition probabilities in a case of the emission and absorption spectrum of nucleus ^{186}Re ($E^{(0)}_{\gamma}$ = 186.7 keV) in the molecule of ReO_4. the main difficulty during calculating corresponding matrix elements is connected with definition of the values $b_{s\sigma}$ of the normalized shifts of **γ**- active decay. It is known that if a molecule has the only normal vibration of the given symmetry type, then the corresponding values of $b_{s\sigma}$ can be found from the well known Eccart conditions, normalization one and data about the molecule symmetry.

1. Introduction

Any alteration of the molecular state must be manifested in the quantum transitions, for example, in a spectrum of the γ-radiation of a nucleus. It is well known that it is possible the transfer of part of a nuclear energy to atom or molecule under radiating (absorption) the γ quanta by a nucleus (c.f.[1-36]). A spectrum contains a set of the electron-vibration-rotation satellites, which are due to an alteration of the state of system interacting with photon. A mechanism of forming satellites in the molecule is connected with a shaking of the electron shell resulting from the interaction between a nucleus and γ quantum. This paper is going on our studying the co-operative dynamical phenomena (c.f.[6б7]) due the interaction between atoms, ions, molecule electron shells and nuclei nucleons. A consistent quantum- mechanical approach to calculation of the electron-nuclear γ transition spectra of a nucleus in the multiatomic molecules has been earlier proposed [2-5]. It generalizes the well known Letokhov-Minogin model [2]. Estimates of the vibration-nuclear transition probabilities in a case of the emission and absorption spectrum of nucleus ^{188}Os in the OsO_4 and ^{191}Ir in the IrO_4 were listed . Here we present the first accurate data on the vibration-nuclear transition probabilities in a case of the emission and absorption spectrum of the nucleus ^{186}Re ($E^{(0)}_{\gamma}$ = 186.7 keV) in the ReO_4.

2. The electron-nuclear γ transition spectra of nucleus in multi-atomic molecule

As the method of computing is earlier presented in details [2-6], here we consider only by the key topics. Hamiltonian of interaction of the gamma radiation with a system of nucleons for the first nucleus can be expressed through the coordinates of nucleons r_n' in a system of the mass centre of one nucleus [2,3]:

$$H(r_n) = H(r_n')\exp(-k_{\gamma}u),$$

where k_{γ} is a wave vector of the γ quantum; u is the shift vector from equality state (coinciding

with molecule mass centre) in system of co-ordinates in the space.

The matrix element for transition from the initial state "a" to the final state "b" is presented as :

$$< \Psi_b^* \mid H \mid \Psi_a > \bullet < \Psi_b^* \mid \hat{a}^{-k_\gamma u} \mid \Psi_a > \qquad (1)$$

where a and b is a set of quantum numbers, which define the vibrational and rotational states before and after interaction (with γ quantum). The first multiplier in (1) is defined by the γ transition of nucleus and is not dependent on an internal structure of molecule in a good approximation.

The second multiplier is the matrix element of transition from the initial state "a" to the final state "b":

$$M_{ba} \propto \Psi_b^*(r_e) \mid \Psi_a(r_e) >$$

$$\bullet < \Psi_b^*(R_1, R_2) \mid e^{-k_\gamma R_1} \mid \Psi_a(R_1, R_2) > \qquad (2)$$

The expression (2) gives a general formula for calculating the probability of changing the internal state of molecule during absorption or emitting γ quantum by a nucleus. It determines an intensity of the corresponding γ-satellites. Their positions are fully determined as:

$$E_\gamma = E_\gamma^0 \pm R + \hbar k_\gamma v \pm (E_b - E_a) .$$

Here M is the molecule mass, v is a velocity of molecule before interaction of nucleus with γ quantum; E_a and E_b are the energies of the molecule before and after interaction; E_γ is an energy of nuclear transition; R_{om} is an energy of recoil:

$$R_{om} = [(E_\gamma^{(o)}]^2 / 2Mc^2.$$

One can suppose that only single non-generated normal vibration (vibration quantum $\hbar\omega$) is excited and initially a molecule is on the vibrational level $v_a = 0$. If we denote a probability of the corresponding excitation as $P(v_b, v_a)$ and use expression for shift u of the γ-active nucleus through the normal co-ordinates, then an averaged energy for excitation of the single normal vibration is as follows:

$$\overline{E}_{vib} = \sum_{v=0}^{\infty} \hbar\omega\left(v + \tfrac{1}{2}\right)\overline{P}(v,0) - \hbar\infty/2 =$$

$$= \sum_{v=0}^{\infty} \hbar\omega\left(v + \tfrac{1}{2}\right)P(v,0) - \hbar\omega/2 =$$

$$= \sum_{v=0} \hbar\omega\left(v + \tfrac{1}{2}\right)\frac{z^v}{v!}e^{-z} - \frac{\hbar\omega}{2} = \frac{1}{2}R\left(\frac{M-m}{m}\right), \qquad (3)$$

where

$$z = (R/\hbar\omega)[M - m/m]\cos^2\vartheta,$$

and m is the mass of γ-active nucleus, ϑ is an angle between nucleus shift vector and wave vector of γ-quantum and line in $\overline{E}_{vib}$ means averaging on orientations of molecule (or on angles ϑ). To estimate an averaged energy for excitation of the molecule rotation, one must not miss the molecule vibrations as they provide non-zeroth momentum $L = k_v \sin\vartheta$, which is transferred to a molecule by γ-quantum. In supposing that a nucleus is only in the single non-generated normal vibration and vibrational state of a molecule is not changed $v_a = v_b = 0$, one could evaluate an averaged energy for excitation of the molecule rotations as follows:

$$\overline{E}_{rot} = \left\langle \overline{BL^2} \right\rangle = Bk_\gamma^2 \left\langle u^2 \right\rangle \overline{\sin^2\vartheta} = \tfrac{1}{2}R(B/\hbar\omega)[(M-m)/m] \qquad (4)$$

A shift u of the γ-active nucleus can be expressed through the normal co-ordinates $Q_{s\sigma}$ of a molecule:

$$u = \frac{1}{\sqrt{m}} \sum_{s\sigma} b_{s\sigma} Q_{s\sigma} \qquad (5)$$

where m is a mass of the γ-active nucleus; components of the vector $b_{s\sigma}$ of nucleus shift due to the σ-component of "s" normal vibration of a molecule are the elements of matrix b [2]; it realizes the orthogonal transformation of the normal co-ordinates matrix Q to matrix of masses of the weighted Cartesian components of the molecule nuclei shifts q. According to (2), the matrix element can be written as multiplying the matrix elements on molecule normal vibration, which takes contribution to a shift of the γ-active nucleus:

$$M(b,a)=\prod_s\left\langle v_s{}^b \mid \prod_\sigma \exp(-k_\gamma b_{s\sigma}Q_{s\sigma}/\sqrt{m})v_s{}^a\right\rangle. \quad (6)$$

It is obvious that missing molecular rotations means missing the rotations which are connected with the degenerated vibrations. Usually wave functions of a molecule can be written for non-degenerated vibration as:

$$|v_s\rangle=\Phi_{v_s}(Q_s),$$

for double degenerated vibration as

$$|v_s\rangle=(v_s+1)^{-1/2}\sum_{v\sigma_1,v\sigma_2,v\sigma_3}\Phi_{v_{s\sigma_1}}(Q_{s\sigma_1})\Phi_{v_{s\sigma_2}}(Q_{s\sigma_2})$$

where $v_{s\sigma_1}+v_{s\sigma_2}=v_s$ and analogously for triple degenerated vibration. In the simple approximation function $\Phi_{v_{s\sigma}}(Q_{s\sigma})$ can be chosen in a form of the linear harmonic oscillator one. More exact calculating requires a numerical determination of these functions. Taking directly the wave functions $|v_s^a\rangle$ and $|v_s^b\rangle$, calculating the matrix element (6) is reduced to a definition of the matrix elements on each component **γ** of the normal vibration.

3. Results and conclusions

Below we present the advanced data on the vibration-nuclear transition probabilities in a case of the emission and absorption spectrum of nucleus ^{191}Ir ($E^{(0)}_\gamma$ = 82 keV) in the molecule IrO_4. Note that the main difficulty during calculating (6) is connected with definition of the values $b_{s\sigma}$- of the normalized shifts of **γ**-active decay. It is known that if a molecule has the only normal vibration of the given symmetry type, then the corresponding values of $b_{s\sigma}$ can be found from the well known Eccart conditions, normalization one and data about the molecule symmetry. For several normal vibrations of the one symmetry type, a definition of $b_{s\sigma}$ requires solving the secular equation for molecule $|GF-\lambda E|=0$. We have used the results of advanced theoretical calculating electron structure of the studied system within an advanced relativistic scheme of the X_α- scattered waves method (see details in Refs.[21-23]). In table 1 we present the results of calculating probabilities of the first several vibration-nuclear transitions in a case of the emission and absorption spectrum of nucleus the nucleus ^{186}Re ($E^{(0)}_\gamma$ = 186.7 keV) in the ReO_4.

Table 1

Probabilitites of the vibrational-nuclear transitions in spectrum of the ReO_4.

Vibration transition $v_3{}^a, v_4{}^a - v_3{}^b, v_4{}^b$	$\overline{P}(v_3{}^a, v_4{}^a - v_3{}^b, v_4{}^b)$
0,0 – 0,0	0.74
1,0 – 0,0	0.014
0,1 – 0,0	0.067
1,0 – 1,0	0.68
0,1 – 0,1	0.61

References

1. Letokhov V. S., Laser Spectroscopy, Academic Press, N.-Y., 1997.
2. Letokhov V.S., Minogin V., Spectrum of gamma transitions of a nucleus in symmetric polyatomic molecule// JETP.-1995.-Vol.69.-P.1569-1581.
3. Glushkov A.V., Khetselius O.Y., Malinovskaya S.V., Spectroscopy of cooperative laser-electron nuclear effects in multiatomic molecules// Molec. Phys.-2008. -Vol.106.-N9-10.-P.1257-1260.
4. 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.
5. Glushkov A.V., Khetselius O.Yu., Svinarenko A.A., Prepelitsa G.P. , Shakhman A., Spectroscopy of cooperative laser-electron nuclear processes in diatomic and multiatomic molecules//Spectral Lines Shape (AIP, USA).-2010.-

Vol.16.-P.269-273.
6. Glushkov A.V., Kondratenko P.A., Buyadzhi V., Kvasikova A.S., Shakhman A., Sakun T., Spectroscopy of cooperative laser electron-γ-nuclear processes in polyatomic molecules// Journal of Physics: C Series (IOP, London, UK).-2014.-Vol.548.-P. 012025 (5p.).
7. Glushkov A.V., Kondratenko P.A., Lopatkin Yu., Buyadzhi V., Kvasikova A., Spectroscopy of cooperative laser electron- γ -nuclear processes in diatomics and multiatomic molecules // Photoelectronics.-2014.-Vol.23.-P.142-146.
8. 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.Brändas, G.Delgado-Barrio (Springer).-2015-Vol.29.-P.55-76.
9. 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.217-229.
10. 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.
11. Khetselius O., Spectroscopy of cooperative electron-gamma-nuclear processes in heavy atoms: NEET effect// J. Phys.: Conf. Ser.-2012.- Vol.397.-P.012012
12. 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.
13. 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.
14. Glushkov A.V., Khetselius O., Svinarenko 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.
15. Glushkov A.V., Khetselius O.Yu., Prepelitsa G., 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 International Geometry Center".-2013.-Vol.6, N1.-P.43-48.
16. 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.
17. Malinovskaya S.V., Glushkov A.V., Khetselius O.Yu., Lopatkin Yu., Loboda A., Svinarenko 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,N2.-P.288-296.
18. Malinovskaya S.V., Glushkov A.V., Khetselius O.Yu., Svinarenko A.A., Mischenko E.V., Florko T.A., Optimized 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.
19. Glushkov A.V., Khetselius O.Yu., Svinarenko A., Prepelitsa G., Mischenko E., 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.
20. 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.
21. Glushkov A.V., Relativistic and correlation effects in spectra of atomic systems.-Odessa: Astroprint.-2006.-400P.
22. Glushkov A.V., Atom in electromagnetic field.-Kiev: KNT, 2005.-450P.
23. Khetselius O.Yu., Hyperfine structure of atomic spectra.-Odessa: Astroprint, 2008.-210P.
24. Khetselius O.Yu., Hyperfine structure of radium// Photoelectronics.-2005.-N14.-P. 83-85.
25. 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, F.Hanappe, Singapore: World Scientific.-2003.-P.242-250.
26. Glushkov A.V., Lovett L., Khetselius O., Gurnitskaya E., Dubrovskaya Yu., Loboda A., 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.
27. 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.
28. 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.
29. 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.
30. 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.
31. Glushkov A.V., Effective quasi-particle valence hamiltonian of molecules in the comprehensive semi-empirical theory// Sov. Journ. Str. Chem.-1998.-Vol.29,N4.-P.3-9.
32. Khetselius O.Yu., Quantum Geometry: New approach to quantization of the quasistationary states of Dirac equation for super heavy ion and calculating hyper fine structure parameters// Proc. Int. Geometry Center.-2012.-Vol.5,№ 3-4.-P.39-45.
33. 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.

34. Gedasimov V N, Zelenkov A G, Kulakov V M et al 1994 *JETP.* **86** 1169; Soldatov A A 1983 Preprint of I.V.Kurchatov Institute for Atomic Energy IAE-3916, Moscow
35. 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.
36. 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. J. Quantum Chem..-2009.-Vol.109, N14.-P.3473-3481.

This article has been received in May 2017.

UDC 539.186

Yu. V. Dubrovskaya, A. A. Kuznetsova, A. S. Kvasikova, T. N. Sakun

SPECTROSCOPY OF COOPERATIVE ELECTRON-γ-NUCLEAR EFFECTS IN MULTIATOMIC MOLECULES: MOLECULE XY_4

Summary

The consistent quantum approach to calculating the electron-nuclear γ transition spectra (a set of the vibration-rotational satellites in a molecule) of a nucleus in the multiatomic molecules is used to get the accurate spectroscopic data on the vibration-nuclear transition probabilities in a case of the emission and absorption spectrum of nucleus ^{186}Re ($E^{(0)}_{\gamma}$= 186.7 keV) in the molecule of ReO_4. the main difficulty during calculating corresponding matrix elements is connected with definition of the values $b_{s\gamma-}$ of the normalized shifts of γ-active decay. It is known that if a molecule has the only normal vibration of the given symmetry type, then the corresponding values of $b_{s\gamma}$ can be found from the well known Eccart conditions, normalization one and data about the molecule symmetry.

Key words electron-nuclear γ transition spectra, vibration-nuclear transition probabilities

УДК 539.186

Ю. В. Дубровская, А. А. Кузнецова, А. С. Квасикова, Т. Н. Сакун

СПЕКТРОСКОПИЯ КООПЕРАТИВНЫХ ЭЛЕКТРОН-ГАММА-ЯДЕРНЫХ ЭФФЕКТОВ В МНОГОАТОМНЫХ МОЛЕКУЛАХ: МОЛЕКУЛА XY_4

Резюме

Последовательный квантовый подход к вычислению спектров электронно-гамма-ядерных переходов (набора колебательно-вращательных сателлитов в молекуле) в многоатомных молекулах применен к определению спектроскопических данных о вероятностях колебательно-

ядерных переходов при излучении и поглощении ядра ^{186}Re ($E^{(0)}_{\gamma}$= 186.7 кэВ) в молекуле ReO_4. Основная трудность при оценке соответствующих матричных элементов связана с определением значений $b_{s\gamma\text{-}}$ нормированных сдвигов гамма-активного распада. Известно, что если молекула имеет единственное нормальное колебание данного типа симметрии, то соответствующие значения $b_{s\gamma\text{-}}$ могут быть найдены из хорошо известных условий Эккарта, условия нормировки и данных о симметрии молекулы.

Ключевые слова: электронно-гамма-ядерный спектр, вероятность колебательно-ядерных переходов

УДК 539.186

Ю. В. Дубровська, Г. О. Кузнецова, Г. С. Квасикова, Т. М. Сакун

СПЕКТРОСКОПІЯ КООПЕРАТИВНИХ ЕЛЕКТРОН-ГАММА-ЯДЕРНИХ ЕФЕКТІВ В БАГАТОАТОМНИХ МОЛЕКУЛАХ: МОЛЕКУЛА XY_4

Резюме

Послідовний квантовий підхід до обчислення спектрів електронно-гамма-ядерних переходів (набору колебательно-обертальних сателітів в молекулі) в багатоатомних молекулах застосований до визначення спектроскопічних даних про ймовірності колебательно-ядерних переходів при випромінюванні і поглинанні ядра ^{186}Re ($E^{(0)}_{\gamma}$= 186.7 кеВ) в молекулі ReO4. Основні труднощі при оцінці відповідних матричних елементів пов’язана з визначенням значень $b_{s\gamma\text{-}}$ – нормованих зрушень гамма-активного розпаду. Відомо, що якщо молекула має єдине нормальне коливання даного типу симетрії, то відповідні значення $b_{s\gamma\text{-}}$ – можуть бути знайдені з добре відомих умов Еккарта, умови нормування і даних про симетрію молекули.

Ключові слова: електрон-гамма-ядерний спектр, ймовірність коливально-ядерних переходів

PACS 73.40.Gk, Lq; 73.61.Ga

Ie.V. Brytavskyi[1], A.V. Tereshchenko[1], V.B. Myndrul[1], M.M. Pavlenko[1,2], V.A. Smyntyna[1]

APPLICATION OF SILICON PILLAR-NANOSTRUCTURES WITH ZINC AND TITAN OXIDES COVERAGE FOR SOLAR ENERGY AND BIOSENSOR DEVICES

[1]Odessa I. I. Mechnikov National University, 2, Dvoryanskaya str., Odessa, 65082, Ukraine
[2]NanoBioMedical Centre, Adam Mickiewicz University, Umultowska 85, Poznan, Poland
Phone: +380(48)7266356, Fax: +380(48)7233461, e-mail: brytav@ukr.net

The work is focused on technology and characterization issues of silicon pillar nanostructures in combination with metal oxides, such as ZnO and TiO_2, for various applications in field of biosensor and solar energy. The metal-assisted chemical etching method (MACE) modified with latex nanobeads lithography and spin-coating technique, was used to fabricate the uniform silicon nanopillar arrays. Atomic layer deposition technique (ALD) which is utilized for formation of oxide layers displays uniform coverage of the arrays and provides thin film formation independently on surface peculiarities. Therefore, it can be applied both for planar samples and 3D patterned substrates with porous media.

Introduction

The technological processing and investigation on nanostructured silicon and its composites with TiO_2 and ZnO, for use in solar energy and biosensing was performed by our group. As a basic material for the research, it was decided to use nanostructured silicon pillars, which could be fabricated with porous surface and, thus, significantly increase the effective area of the interaction, which is a crucial factor for use in biosensing approach.

Application of silicon nanopillars, especially with porous surface, can be implemented in the form of optical or electro-physical detection of molecules, including complex biomolecules.

Resent data published in literature demonstrate the advantage of the column structure compared to conventional porous substrate [1-3]. The contact area for molecule detection is fixed depending on changes in the electrical conductivity of the sensor material. The usage of arrays with parallel oriented nanopillars could reduce the signal-to-noise ratio, and thereby increase the sensitivity of the sensor [4].

The next prospective application for arrays of aligned silicon nanopillars is utilization for high efficiency solar cells. The main principle is based on irradiation of radial p-n junction obtained on silicon nanopillar coated by semiconductor material. In this approach any semiconductor may be used but silicon is an obvious choice due to low cost and relatively simple processing. In case of nanowires the quantum confinement effect is more noticeable and utilization of silicon more profitable, taking into account triviality and readiness of chemical methods, such as electrochemical and metal-assisted etching [5].

One of the prominent applications of wire/pillar based structures is a photoanode material in the process of water splitting, the separation of water into H_2 and O_2 under the sunlight. Currently promising option in this direction is the using of n-type silicon contact with n-type titanium dioxide, where charge carriers concentration could be increased by additional N-doping. Therefore, using of TiO_2 or ZnO nanocomposite structure can greatly improve the quality of the photoanode.

Silicon nano-pillars technology

The process of fabrication of aligned silicon nanopillar arrays is based on the method called metal-assisted chemical etching (MACE), which was studied by our research group in recent years [6-8].

A chemical treatment of silicon implies a top-down approach and realized by silicon wafer

etching in a solution of hydrofluoric acid and oxidizing agent (hydrogen peroxide in this research). To control the morphology of Si wafer the mask of polystyrene nanobeads (about 800 nm) was deposited onto the hydrophilic silicon surface. Hydrophilicity was achieved by RCA treatment which is a standard process for cleaning of silicon wafers. After obtaining of nanobead monolayer the reactive ion etching in oxygen atmosphere was applied for convergence of the nanosphere sizes up to 600 nm. Photoelectron lithography could be used with the same success but our approach is faster and comparatively cheaper.

A thin layer of gold was used as a catalyst. Any of the noble metals could be used in this process, but the only difference lays in the dynamics of etching and peculiarities of chemical reactions.

During the practical implementation of the MACE method, it was solved a number of technical problems related to the formation of the nanospheres monolayer, the dynamics of the etching process, and so on.

The fabrication features

SEM images show a periodic structure of nanopillar arrays fabricated onto p-type silicon wafer (Fig. 1). Due to crucial influence on the etching process, which exerts by holes, the porous nanopillars could be obtained much easier for p-type Si. However, for the n-type Si it is possible to choose conditions that can be also leading to the formation of a porous structure. For the n-type Si the peculiarities of the surface processes, including barrier properties at the interface silicon – etching solution are very important. With sufficient electron density and presence of bending zones at the interface, the etching process occurs even more intensive than for p-type silicon. These conditions are achievable by increasing the concentration of oxidizers that leads to increasing of the silicon oxidation rate.

Formation of the nanobead monolayer is the first important technological stage. It can be achieved by the spin-coating technique under high-speed rotation of the substrate. According to nanosphere size and total area of the sample this stage may be consisted of few successive steps with different rotation rates.

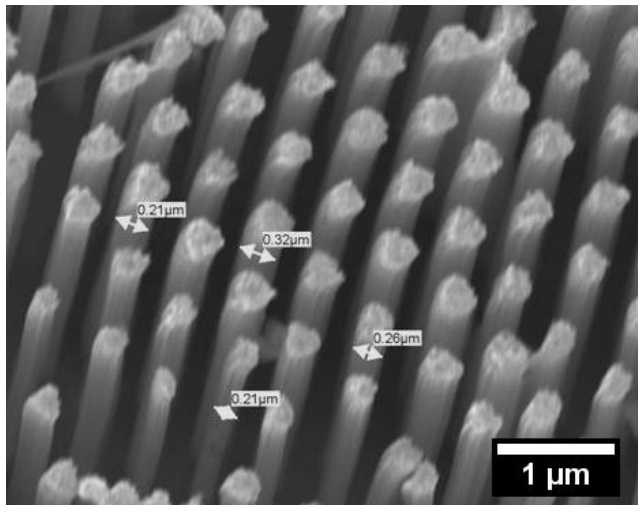


Fig 1. Nanopillar arrays fabricated on p-type silicon wafer

Figure 2 a shows SEM image of formed self-ordered monolayer, the border and point defects are clearly seen. Almost defect-free film is forming after adding methanol into the nanobeads solution before the spin-coating process. The obtained film shows quite dense hexagonal packing that is suitable for further processing.

The surface of the silicon after reactive ion etching in the oxygen plasma and deposition of a gold layer by magnetron sputtering is shown in Fig. 2 b, partially sphere removed surface shows the final etching pattern. The coated area is etching faster and as a result an aligned array of silicon nanopillars is emerging. The nanospheres could be removed in an ultrasonic bath by placing the sample in ethanol.

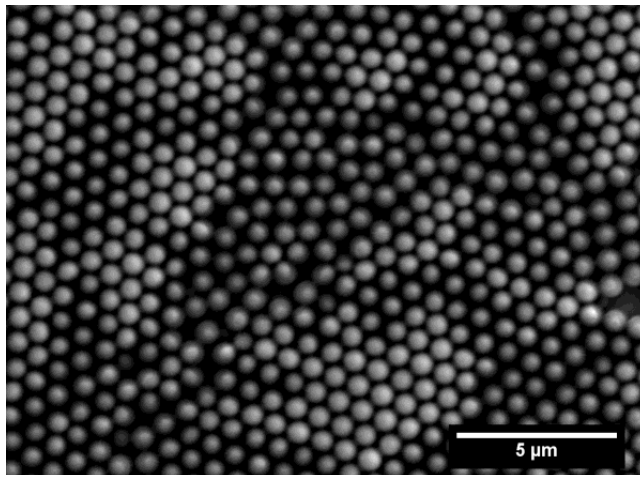


Fig. 2 a. SEM image of formed self-ordered monolayer

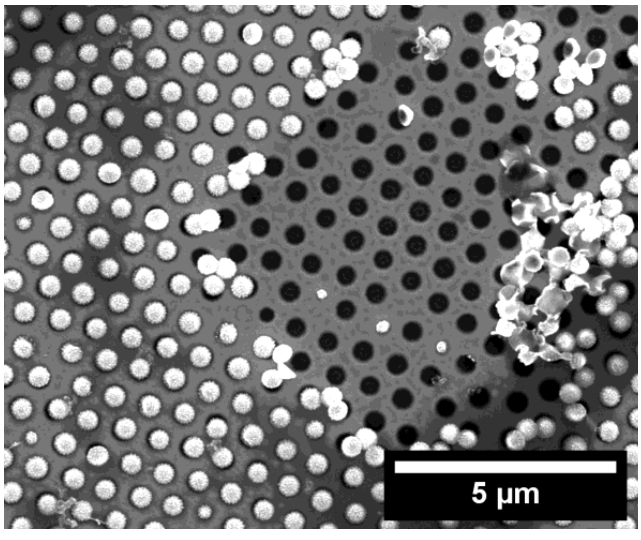


Fig. 2 b. Final etching pattern

As a result of all treatments and subsequent etching the evenly distributed hexagonal straight aligned porous nanopillar arrays are formed. By choosing the etching parameters and conditions a set of samples suitable for subsequent deposition of titanium dioxide and zinc oxide were obtained, and investigation on optical, structural and biosensing properties were performed.

For application of this type of structures in the solar energy the nanopillar arrays with bundle packed structure were obtained. These structures possess a high absorption coefficient due to additional absorption of the radiation reflected from the surface of the substrate. The advantage of such a structure over the conventional vertical arrays described in the literature and is widely studied at the present time [9].

The morphology of an individual nanopillar was investigated in details. For this purpose nanopillar arrays was decomposed in ultrasonic bath and investigated by SEM. The porous surface of a single pillar is shown in Fig. 3. The pore size is about 10-20 nm and relate to mesopores. Thorough investigation has shown that at least for the p-type Si a microporous structure with scale of 2 - 8 nm could be formed.

The ability of controlling the comprehensive morphology on pillar-structure, such as height, diameter and pore size allows us to consider these periodic nanopillar arrays as a promising material for continuing the research of silicon nanocomposite structures application for biosensor devices [10].

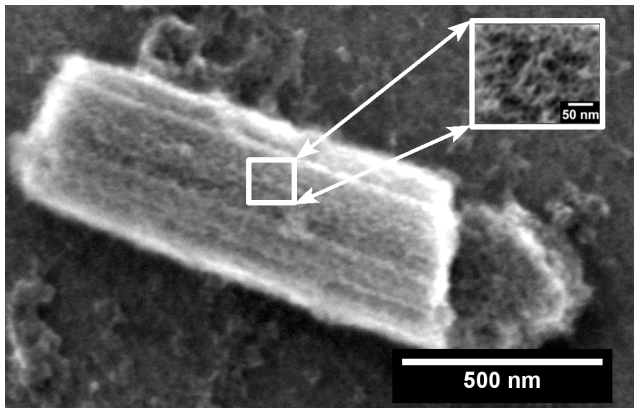


Fig. 3. Surface of a single pillar

The bulk material of the nanopillars also demonstrates a porous structure as it can be seen from "stump" of a single nanopillar (Fig. 4), also the same structure pertains to the surrounding region (silicon substrate).

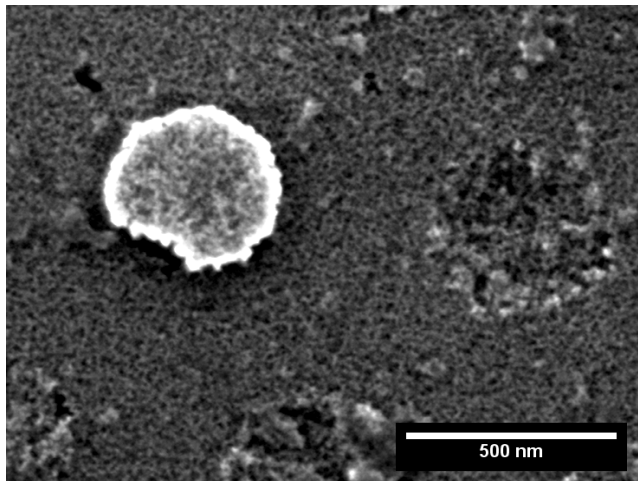


Fig. 4. Stump of a single nanopillar

Characterization of metal oxide layers

After fabrication of the aligned nanopillar arrays the next stage is a deposition of titanium dioxide and zinc oxide. Atomic layer deposition (ALD) was used for this purpose [11]. This method uses self-limiting chemical reactions between the precursors. Atomic Layer Deposition technique provides even thin film deposition and can be applied for planar surface, 3D patterned substrate and porous structure [7, 12]. Processing per cycle takes time of few seconds (precursor sputtering in the chamber for less than a second). Typical ALD process involves three stages: inlet

of first precursor, chemical reaction to the surface and blowing off the chamber with nitrogen. Then second precursor goes through the stages the same order.

A complex nanocomposite structure is forming after the deposition of titanium dioxide on the porous nanopillar arrays. At a certain pillar's height and thickness of titanium dioxide layer occurs a mechanical deformation of the array (Fig. 5). In order to investigate this process the TiO_2 layer was deposited in the range of 150 to 500 ALD cycles, the equivalent growth rate for smooth surface is about 0.2 Å per cycle. Mechanical changes in the pillar arrays structure takes place at sufficiently large height and could lead to destruction of the too high pillars. As well a crucial destruction influence on the lengthy pillar arrays occurs during the etching process due to hydrodynamic forces.

Such a complex composite system is very interesting for future research, including features of quantum confinement effects and application in biosensor devices.

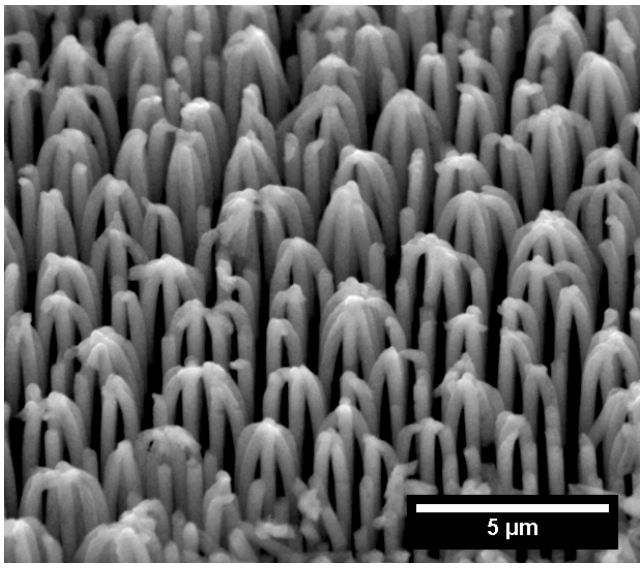


Fig. 5. Mechanical deformation of the array

By filling the space between pillars, TiO_2 forms an amorphous photoactive layer, which provides an effective light harvesting on the heterojunction interface. During the ALD process, TiO_2 quite deeply penetrates into the pores and additional annealing process induces a complex polycrystalline structure in the matrix of porous silicon.

The similar nanocomposite based on ZnO was also investigated for biosensor application. The principle of operation of the biosensor is based on immobilization of the biosensitive layer on the surface of zinc oxide [8, 10]. Presence of the detected substance could be estimated through reflectivity or luminescence spectra due to surface plasmon resonance effect under UV irradiation. Probes of ZnO/Si nanolaminates were fabricated for investigation of this process. Deposition of 250 and 500 ZnO ALD cycles were implemented onto flat silicon substrate. Obtained probes have shown a good stability and high adhesion, therefore further investigation of mentioned composite structures seems to be prospective.

Results and conclusion

Thus, an important problem was resolved – identification and optimization of new and known technological mechanisms in nanosilicon forming processes that have influence on the optical, structural and surface properties of obtained Si / ZnO and Si / TiO_2 nanocomposites as a result of the influence of components interaction and external factors with the aim of stabilization of the properties of materials based on nanocomposite materials.

The technology of porous silicon nanopillars and new nanocomposites based on the method of using chemical nonelectrolytic etching and atomic layered deposition was developed. Structural characteristics of the obtained complex nanocomposite structures were determined by using of SEM equipment.

On the base of the described approach of nanosilicon composites in modern electronic industry the properties of existing photosensitive, gas-sensitive and other media can be improved, and also the improvement of operating parameters of devices on the base of nanopillar Si with a simultaneous reduction in the cost of raw materials which may lead to lower the prices of mentioned devices. The research results can be used in the development of applied sections of surface physics, semiconductor physics, materials science, micro- and nanoelectronics. Technological optimization results can be used in developed processes to create nanostructures on silicon. Theoretical information and new fundamental results on optical and electrical properties of nanoscale systems, such as studied Si nanopillars, give the

way to perform the basic properties research of nano-Si composites, their practical use and creation of new devices electronic technology on its base.

Reference

[1] H. S. Wasisto, S. Merzsch, A. Stranz, A. Waag, E. Uhde, T. Salthammer and E. Peiner, Sens. Actuators, B, 2013, 189, 146–156.

[2] B. D. Choudhury, R. Casquel, M. J. Banuls, F. J. Sanza, M. F. Laguna, M. Holgado, R. Puchades, A. Maquieira, C. A. Barrios and S. Anand,Opt. Mater. Express, 2014, 4, 1345–1354.

[3] M. Kandziolka, J. J. Charlton, I. I. Kravchenko, J. a. Bradshaw, I. a. Merkulov, M. J. Sepaniak and N. V. Lavrik, Anal. Chem., 2013, 85, 9031–9038.

[4] Y. J. Hwang, A. Boukai and P. Yang, Nano Lett., 2009, 3, 410–415.

[5] H. Lin, M. Fang, H.-Y. Cheung, F. Xiu, S. Yip, C.-Y. Wong and J. C. Ho, RSC Adv., 2014, 4, 50081–50085.

[6] I. Iatsunskyi, M. Pavlenko, R. Viter, M. Jancelewicz, G. Nowaczyk, I. Baleviciute, K. Załęski, S. Jurga, A. Ramanavicius, V. Smyntyna, The Journal of Physical Chemistry C 119 (2015) 7164−7171

[7] I. Iatsunskyi, M. Pavlenko, G. Nowaczyk, V. Fedorenko, S. Jurga, V. Smyntyna / Optic. - 2015, 126, 1650-1655

[8] A.V. Tereshchenko, V.A. Smyntyna, I.P. Konup, S.A. Geveliuk, M.F. Starodub, Springer Science+Business Media Dordrecht 2016, Nanomaterials for Security, NATO Science for Peace and Security Series A: Chemistry and Biology, 2016

[9] Dong-Myeong Shin, Hye Ji Han, Won-Geun Kim, Eunjong Kim, Chuntae Kim, Suck Won Hong, Hyung Kook Kim, Jin-Woo Oh and Yoon-Hwae Hwang, Energy Environ. Sci., 2015,8, 3198-3203

[10] A. Tereshchenko, M Bechelany, R. Viter, V. Khranovskyy, V. Smyntyna, N. Starodub, R. Yakimova, Sensors and Actuators B 229 (2016) 664–677.

[11] Y. Yan, D. Wang and P. Schaaf, Dalton Trans., 2014, 43, 8480–8485.

[12] R. Viter, I. Iatsunskyi, V. Fedorenko, S. Tumenas, Z. Balevicius, A. Ramanavicius, S. Balme, M. Kempin, G. Nowaczyk, S. Jurga and M. Bechelany, J. Phys. Chem. C, 2016,120, 5124–5132.

Article received on May 2017

PACS 73.40.Gk, Lq; 73.61.Ga

Ie. V. Brytavskyi, A. V. Tereshchenko, V. B. Myndrul, M. M. Pavlenko, V. A. Smyntyna

SILICON NANOPILLARS FORMING AND COVERING BY Zn AND Ti OXIDES FOR SOLAR ENERGY APPLICATIONS AND BIOSENSORICS

Summary

The work is focused on technology and characterization issues of silicon pillar nanostructures in combination with metal oxides, such as ZnO and TiO_2, for various applications in field of biosensor and solar energy. The metal-assisted chemical etching method (MACE) modified with latex nanobeads lithography and spin-coating technique, was used to fabricate the uniform silicon nanopillar arrays. Atomic layer deposition technique (ALD) which is utilized for formation of oxide layers displays uni-

form coverage of the arrays and provides thin film formation independently on surface peculiarities. Therefore, it can be applied both for planar samples and 3D patterned substrates with porous media.

Key words: nanopillars, atomic layer deposition, nanocomposites

УДК 73.40.Gk, Lq; 73.61.Ga

Є. В. Бритавський, А. В. Терещенко, В. Б. Миндрул, М. М. Павленко, В. А. Сминтина

ФОРМУВАННЯ КРЕМНІЄВИХ НАНО-ПІЛЛАРСІВ ТА ПОКРИТТЯ ЇХ ОКСИДАМИ ЦИНКУ ТА ТИТАНУ ДЛЯ ВИКОРИСТАННЯ В СОНЯЧНІЙ ЕНЕРГЕТИЦІ ТА БІОСЕНСОРИЦІ

Анотація

Робота присвячена технології і характеризації кремнієвих наноструктур в поєднанні з покриттям оксидами металів для різних застосувань в біосенсориці і сонячній енергетиці. У статті описується спосіб неелектролітичного травлення, модифікованого використанням шару наносфер на підкладці, сформованого методом поверхневого центрифугування. Метод атомно-шарового осадження, який використовувався для формування оксидів на наноструктурах, демонструє утворення рівномірного шару і не залежить від геометрії підкладки, тому він може застосовуватися як для плоских зразків, так і для підкладок з тривимірною структурою і з пористими шарами.

Ключові слова: наностовбчик, атомно-шарове осадження, нанокомпозит

УДК 73.40.Gk, Lq; 73.61.Ga

Е. В. Бритавский, А. В. Терещенко, В. Б. Мындрул, Н. Н. Павленко, В. А. Смынтына

ФОРМИРОВАНИЕ КРЕМНИЕВЫХ НАНО-ПИЛЛАРСОВ И ПОКРЫТИЯ ИХ ОКСИДАМИ ЦИНКА И ТИТАНА ДЛЯ ИСПОЛЬЗОВАНИЯ В СОЛНЕЧНОЙ ЭНЕРГЕТИКЕ И БИОСЕНСОРИКЕ

Аннотация

Работа посвящена технологии и характеризации кремниевых наноструктур в сочетании с оксидами металлов для различных применений в биосенсорике и солнечной энергетике. В статье описывается способ неэлектролитического травления, модифицированного использованием слоя наносфер на подложке, сформированного методом поверхностного центрифугирования. Метод атомно-слоевого осаждения, который использовался для формирования оксидов на наноструктурах, демонстрирует образование равномерного слоя и не зависит от геометрии подложки, поэтому он может применяться как для плоских образцов, так и для подложек с трехмерной структурой и с пористыми слоями.

Ключевые слова: наностолбик, атомно-слоевое осаждение, нанокомпозит

UDC 539.182

I. N. Serga, O. Yu. Khetselius, L. A. Vitavetskaya, A. N. Bystryantseva

Odessa National Polytechnical University, 1, Shevchenko pr.,1, Odessa, 65044
Odessa State Environmental University, 15, Lvovskaya str., Odessa, 65016
e-mail: vitavetskayala@gmail.com

RELATIVISTIC THEORY OF SPECTRA OF PIONIC ATOMIC SYSTEMS ^{208}Pb WITH ACCOUNT OF STRONG PION-NUCLEAR INTERACTION EFFECTS

It is presented a consistent relativistic theory of spectra of the pionic atoms on the basis of the Klein-Gordon-Fock with a generalized radiation and strong pion-nuclear potentials. It is applied to calculation of the energy and spectral parameters for pionic atoms of the 208Pb with accounting for the radiation (vacuum polarization), nuclear (finite size of a nucleus) and the strong pion-nuclear interaction corrections. The measured values of the Berkley, CERN and Virginia laboratories and alternative data based on other versions of the Klein-Gordon-Fock theories with taking into account for a finite size of the nucleus in the model uniformly charged sphere and the standard Uehling-Serber radiation correction and optical atomic theory are listed too. There are listed new data on shift and broadening of the 4f level in 208Pb due to the strong pion-nuclear interaction.

1. Introduction

In papers [1-3] we have presented a new relativistic method of the Klein-Gordon-Fock equation with an generalized pion-nuclear potential to determine transition energies in spectroscopy of light, middle and heavy pionic atoms with accounting for the strong interaction effects. In this paper, which goes on our studying on spectroscopy of pionic atoms, we firstly applied method [1-3] to calculating calculation of the energy and spectral parameters for pionic atom of the ^{208}Pb with accounting for the radiation (vacuum polarization), nuclear (finite size of a nucleus) and the strong pion-nuclear interaction corrections. There are listed new data on shift and broadening of the 4f level in ^{208}Pb due to the strong pion-nuclear interaction.

Following [1-3], let us remind that spectroscopy of hadron atoms has been used as a tool for the study of particles and fundamental properties for a long time. Exotic atoms are also interesting objects as they enable to probe aspects of atomic and nuclear structure that are quantitatively different from what can be studied in electronic or "normal" atoms. At present time one of the most sensitive tests for the chiral symmetry breaking scenario in the modern hadron's physics is provided by studying the exotic hadron-atomic systems. Nowadays the transition energies in pionic (kaonic, muonic etc.) atoms are measured with an unprecedented precision and from studying spectra of the hadronic atoms it is possible to investigate the strong interaction at low energies measuring the energy and natural width of the ground level with a precision of few meV [1-20]. The strong interaction is the reason for a shift in the energies of the low-lying levels from the purely electromagnetic values and the finite lifetime of the state corresponds to an increase in the observed level width. For a long time the similar experimental investigations have been carried out in the laboratories of Berkley, Virginia (USA), CERN (Switzerland). The most known theoretical models to treating the hadronic (pionic, kaonic, muonic, antiprotonic etc.) atomic systems are presented in refs. [21-48]. The most difficult aspects of the theoretical modeling are reduced to the correct description of pion-nuclear strong interaction [1-3] as the electromagnetic part of the problem is reasonably accounted for.

2. Relativistic approach to pionic atoms spectra

As the basis's of a new method has been published, here we present only the key topics of an approach [1-3]. All available theoretical models to treating the hadronic (kaonic, pionic) atoms are naturally based on the using the Klein-Gordon-Fock equation [2,5], which can be written as follows :

$$m^2c^2\Psi(x) = \{\frac{1}{c^2}[i\hbar\partial_t + eV_0(r)]^2 + \hbar^2\nabla^2\}\Psi(x) \quad (1)$$

where c is a speed of the light, *h* is the Planck constant, and $\Psi_0(x)$ is the scalar wave function of the space-temporal coordinates. Usually one considers the central potential [$V_0(r)$, 0] approximation with the stationary solution:

$$\Psi\,(x) = \exp(-iEt/\hbar)\,\varphi(x)\,, \quad (2)$$

where $\varphi(x)$ is the solution of the stationary equation:

$$\{\frac{1}{c^2}[E + eV_0(r)]^2 + \hbar^2\nabla^2 - m^2c^2\}\varphi(x) = 0 \quad (3)$$

Here E is the total energy of the system (sum of the mass energy mc^2 and binding energy ε_0). In principle, the central potential V_0 naturally includes the central Coulomb potential, the vacuum-polarization potential, the strong interaction potential. The most direct approach to treating the strong interaction is provided by the well known optical potential model (c.g. [2]). The nuclear potential for the spherically symmetric density $\rho(r|R)$ is [13-15]:

$$V_{nucl}(r|R) = -((1/r)\int_0^r dr'r'^2\rho(r'|R) + \int_r^\infty dr'r'\rho(r'|R) \quad (4)$$

The most popular Fermi-model pproximation the charge distribution in the nucleus $\rho(r)$ is:

$$\rho(r) = \rho_0\,/\{1 + \exp[(r-c)/a)]\}, \quad (5)$$

where the parameter *a=0.*523 fm, the parameter *c* is chosen by such a way that it is true the following condition for average-squared radius:

$$<r^2>^{1/2}=(0.836\cdot A^{1/3}+0.5700)\text{fm}.$$

The effective algorithm for its definition is used in refs. [12] and reduced to solution of the following system of the differential equations with the corresponding boundary conditions. Another, probably, more consistent approach is in using the relativistic mean-field (RMF) model, which been designed as a renormalizable meson-field theory for nuclear matter and finite nuclei [21]. The detailed presentation of our method for construction of the many-body relativistic perturbation theory with accounting for relativistic, exchange-correlation, nuclqar and radiative (QED) effects is presented in Refs. [41-77]. Here we note that to account QED effect, namely, the vacuum polarization one we have used the generalized Ueling-Serber potential with modification to take into account the high-order corrections.

The most difficult aspect is an adequate account for the strong interaction. On order to describe the strong π^-N interaction we have used the optical potential model in which the generalized Ericson-Ericson potential is as follows:

$$V_{\pi^-N} = V_{opt}(r) = -\frac{4\pi}{2\overline{m}}\left\{q(r)\nabla\frac{\alpha(r)}{1+4/3\pi\xi\alpha(r)}\nabla\right\} \quad (9)$$

$$q(r) = \left(1+\frac{m_\pi}{m_N}\right)\{b_0\rho(r) + b_1[\rho_n(r) - \rho_p(r)]\} + \quad (10)$$

$$+\left(1+\frac{m_\pi}{2m_N}\right)\{B_0\rho^2(r) + B_1\rho(r)\delta\rho(r)\}, \quad (10)$$

$$\alpha(r) = \left(1+\frac{m_\pi}{m_N}\right)^{-1}\{c_0\rho(r) + c_1[\rho_n(r) - \rho_p(r)]\} + \quad (11)$$

Here $\rho_{p,n}(r)$ – distribution of a density of the protons and neutrons, respectively, ξ – parameter ($\xi = 0$ corresponds to case of "no correlation", $\xi = 1$, if anticorrelations between nucleons); respectively isoscalar and isovector parameters b_0, c_0, B_0, b_1, c_1, C_0 B_1, C_1 –are corresponding to the s-wave and p-wave (repulsive and attracting potential member) scattering length in the combined spin-isospin space with taking into account the

absorption of pions (with different channels at p-p pair $B_{0(pp)}$ and *p-n* pair $B_{0(pn)}$), and isospin and spin dependence of an amplitude π-N scattering

$$(b_0\rho(r) \to b_0\rho(r) + b_1\{\rho_p(r) - \rho_n(r)\},$$

the Lorentz-Lorentz effect in the p-wave interaction. For the pionic atom with remained electron shells the total wave-function is a product of the product Slater determinant of the electrons subsystem (Dirac equation) and the pionic wave function. In whole the energy of the hadronic atom is represented as the sum:

$$E \approx E_{KG} + E_{FS} + E_{VP} + E_N; \qquad (12)$$

Here E_{KG} -is the energy of a pion in a nucleus (Z, A) with the point-like charge (dominative contribution in (12)), E_{FS} is the contribution due to the nucleus finite size effect, E_{VP} is the radiation correction due to the vacuum-polarization effect, E_N is the energy shift due to the strong interaction V_N.

The strong pion-nucleus interaction contribution can be found from the solution of the Klein-Gordon-Fock equation with the corresponding pion-nucleon potential. The detailed description and analysis of different aspects of the computational procedure can be found in Refs. [1-4,48-75].

the shift and broadening (keV) of the 4f level due to the strong pion-nuclear interaction [2-8].

Table 1

Transition energies (keV) in the spectra of heavy pionic atom ^{208}Pb (see text)

Trans.	CERN E_{EXP}	E_N [14, 18]	E_N, Our data
4f-3d	1282 ± 2.2	1261.23	1281.78
5g-4f	575.46 ± 0.04	-	575.78

Here we use the short designation of the $V_{\pi N}$: potential parameter sets: Tauscher, -Tau1; Tauscher, -Tau2; Batty etal-Bat .; Seki etal- Sek; Laat-Konijin etal - Laat, Our set – our.

Our parameterization $V_{\pi N}$ upheld options that are the most reliably determined (B_0,c_0,c_1,C_0). The potential parameters whose values differ greatly in different sets, in particular, b_1 (b_1=–0.094) plus not included still to the $V_{\pi N}$ parameter set (ImB_1, ImC_1) were optimized by calculating the strong dependencies shifts for the pionic π^{-20}Ne,^{24}Mg, ^{93}Nb,^{133}Cs,^{175}Lu,^{181}Ta,^{197}Au,^{208}Pb atoms upon the values of b_1, ImB_1,ImC_1; further the selected these

Table 2

Shift and broadening (keV) of the 4f level due to the strong pion-nuclear interaction

ε_{4f},Γ_{4f}	Exp	H-like Func.	Tau1 $\xi = 0$	Tau2 $\xi = 1$	Bat $\xi = 1$	Sek $\xi = 1$	Laat $\xi = 1$	Our $\xi = 1$
^{208}Pb: ε	1.68±0.04	-	1.76	1.62	1.58	1.39	1.68	1.65
^{208}Pb: Γ	0.98±0.05	-	1.18	1.04	1.03	0.86	0.98	0.97

3. Results and conclusions

In table 1 our data on the *4f-3d, 5g-4f* transition energies for pionic atom of ^{208}Pb are presented. The measured values of the CERN and alternative data based on other versions of the Klein-Gordon-Fock theories with taking into account for a finite size of the nucleus in the model uniformly charged sphere and the standard Uehling-Serber radiation correction and optical atomic theory are listed too [2-10]. In table 2 we present data on values meet the standard deviation of the least reliable experimental values.

The analysis of the presented data indicate on the importance of the correct accounting for the radiation (vacuum polarization) and the strong pion-nuclear interaction corrections. Obviously, it is clear that that the contributions provided by the finite size effect should be accounted in a precise theory. Besides, taking into account the increasing accuracy of the X-ray pionic atom spectroscopy experiments, it can be noted that knowl-

edge of the exact electromagnetic theory data will make more clear the true values for parameters of the pion-nuclear potentials and correct the disadvantage of widely used parameterization of the potentials (9)-(11).

References

1. Bystryantseva A.N., Khetselius O.Yu., Dubrovskaya Yu.V., Vitavetskaya L.A., Berestenko A., Relativistic theory of spectra of heavy pionic atomic systems with account of strong pion-nuclear interaction effects: ^{93}Nb, ^{173}Yb, ^{181}Ta, ^{197}Au// Photoelectronics.-2016.-Vol.25.-P.56-61
2. Serga I.N., Dubrovskaya Yu.V., Kvasikova A., Shakhman A.N., Sukharev D.E., Spectroscopy of hadronic atoms: Energy shifts// Journal of Physics: C Ser. (IOP).-2012.- Vol.397.-P.012013 (5p.).
3. Khetselius O.Yu., Hyperfine Structure, scalar-pseudoscalar interaction and parity non-conservation effect in some heavy atoms and ions/ Khetselius O.Yu., Florko T.A., Nikola L.V., Svinarenko A.A., Serga I.N., Tkach T.B., Mischenko E.V. // Quantum Theory: Reconsideration of Foundations (AIP).-2010.-Vol.1232.-P.243-250.
4. Deslattes R., Kessler E., Indelicato P., de Billy L., Lindroth E. , Anton J., Exotic atoms// Rev. Mod. Phys. -2003.-Vol.75.-P.35-70.
5. Scherer S, Introduction to chiral perturbation theory//Advances in Nuclear Physics, Eds. J.W. Negele and E.W. Vogt (Berlin, Springer).-2003.-Vol.27.-P.5-50.
6. Lyubovitskij V., Rusetsky A., πp atom in ChPT: Strong energy-level shift/ // Phys. Lett.B.-2000.-Vol.494.-P.9-13.
7. Anagnostopoulos D., Biri S., Boisbourdain V., Demeter M., Borchert G. et al-PSI, Low-energy X-ray standards from pionic atoms/ //Nucl. Inst. Meth.B.-2003.-Vol.205.-P.9-18.
8. Olaniyi B, Shor A, Cheng S., Dugan G., Wu C.S., Electric quadrupole moments and strong interaction effects in piomic atoms of ^{165}Ho, ^{175}Lu, ^{176}Lu,^{179}Hf, ^{181}Ta //Nucl. Phys. A.-1982.-Vol.403.-P.572-588.
9. Serga I., Relativistic theory of spectra of pionic atoms with account of the Radiative and nuclear corrections/ Serga I.N.// Photoelectronics.-2013.-Vol.22.-P.84-92.
10. Kolomeitsev E.E., Kaiser N., Weise W. Chiral dynamics of deeply bound pionic atoms/ //Phys. Rev. Lett.-2003.-Vol.90.-P.092501.
11. Khetselius O.Yu., Hyperfine structure of atomic spectra.- Odessa: Astroprint, 2008.-210P.
12. Khetselius O.Yu., Hyperfine structure of radium// Photoelectronics.-2005.-N14.-P.83-85.
13. Khetselius O., Spectroscopy of cooperative electron-gamma-nuclear processes in heavy atoms: NEET effect// J. Phys.: Conf. Ser.-2012.- Vol.397.-P.012012
14. 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.
15. 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.
16. 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.
17. 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.
18. Glushkov A.V., Khetselius O.Y., Brusentseva S.V., Zaichko P.A., Ternovsky

V.B., Studying interaction dynamics of chaotic systems within a non-linear prediction method: application to neurophysiology// Advances in Neural Networks, Fuzzy Systems and Artificial Intelligence, Ser: Recent Adv. in Computer Engineering, Ed. J.Balicki.-2014.-Vol.21.-P.69-75.

19. Khetselius O.Yu., Quantum Geometry: New approach to quantization of the quasistationary states of Dirac equation for super heavy ion and calculating hyper fine structure parameters// Proc. Int.Geometry Center.-2012.-Vol.5,№ 3-4.-P.39-45.
20. Glushkov A.V., Khetselius O.Yu., Svinarenko A.,Theoretical spectroscopy of autoionization resonances in spectra of lanthanide atoms// Physica Scripta.-2013.-Vol.T153.-P.014029.
21. 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.
22. Khetselius O.Yu., Relativistic calculating the spectral lines hyperfine structure parameters for heavy ions//Spectral Line Shapes, AIP Conf. Proc.-2008.-Vol.1058.-P.363-365.
23. 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. Proc.-2008.-Vol.1058.-P.231-233.
24. Khetselius O.Yu., Hyperfine structure of energy levels for isotopes ^{73}Ge, ^{75}As, ^{201}Hg// Photoelectronics.-2007.-N16.-P.129-132.
25. 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.
26. 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.
27. 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.
28. 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.
29. Glushkov A V, Ambrosov S V, Loboda A V, Chernyakova Yu, Svinarenko A A, Khetselius O Yu, QED calculation of the superheavy elements ions: energy levels, radiative corrections, and hfs for different nuclear models//Journal Nucl. Phys. A.: nucl. and hadr. Phys.-2004.-Vol.734.-P.21
30. Glushkov A.V., Khetselius O.Yu., Kuzakon V., Prepelitsa G.P., Solyanikova E.P., Svinarenko A., Modeling of interaction of the non-linear vibrational systems on the basis of temporal series analyses (application to semiconductor quantum generators)// Dynamical Systems-Theory and Applications.-2011.-BIF110.
31. Svinarenko A.A., Nikola L. V., Prepelitsa G., 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.
32. 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
33. 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.
34. Glushkov A.V., Energy approach to resonance states of compound super-heavy nucleus and EPPP in heavy nucleus collisions// Low Energy Antiproton Phys. AIP Conference Proceedings.-2005.-Vol.796.-P.206-210.
35. Malinovskaya S.V., S.V., Dubrovskaya Yu., Vitavetskaya L., Advanced quantum mechanical calculation of the beta decay probabilities// Low Energy Antiproton Phys. AIP Conf. Proc.-2005.-Vol.796.-P.201-205.
36. 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.
37. 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.
38. 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.
39. 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.
40. 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.
41. Glushkov A.V., Ambrosov S.V., Loboda A.V., Gurnitskaya E.P., Khetselius O.Yu., QED calculation of heavy multicharged ions with account for the correlation, radiative and nuclear effects// Recent Advances in the Theory of Chemical and Physical Systems (Springer).-2006.-Vol.15.-P.285-299.
42. 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.
43. 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 shileding approximation// Sensor Electr. and Microsyst. Techn.-2007.-N2.-P.9-13
44. 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.
45. Glushkov A.V., Bunyakova Yu.Ya., Zaichko P., Geometry of Chaos: Consistent combined approach to treating chaotic dynamics atmospheric pollutants and its forecasting// Proc. International Geometry Center".-2013.-Vol.6, N3.-P.6-14.
46. 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.
47. 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.
48. 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.
49. Serbov N.G., Glushkov A.V., Bunyakova Yu.Ya., Prepelitsa G.P., Svinarenko A.A., Sensing the kinetical features of energy exchange in mixture CO_2-N_2-H_20 of atmospheric gases under interacting with laser radiation// Sensor Electr. and Microsyst. Techn.-2006.-N4.-P.20-22.
50. Glushkov A.V., Khetselius O.Y., Bunyakova Yu.Ya., Prepelitsa G.P., Solyanikova E.P., Serga E., Non-linear prediction method in short-range forecast of atmospheric pollutants: low-dimensional chaos// Dynamical Systems - Theory and Applications (Lodz).-2011.-LIF111.
51. Khetselius O.Yu., Forecasting evolutionary dynamics of chaotic systems using advanced non-linear prediction method// Dynamical Systems – Theory and Applications, Eds. J. Awrejcewicz, M. Kazmierczak, P. Olejnik, J, Mrozowski.-2013.-Vol.1.-P.145-152.
52. Glushkov A.V., Kuzakon V.M., Ternovsky V.B., Buyadzhi V.V., Dynamics of laser systems with absorbing cell and backward-wave tubes with elements of a chaos// Dynamical Systems – Theory and Applications, Eds. J. Awrejcewicz, M. Kazmierczak, P. Olejnik, J, Mrozowski.-2013.-Vol.T1.-P.461-466.
53. Bunyakova Yu.Ya., Khetselius O.Yu., Non-linear prediction statistical method in forecast of atmospheric pollutants// Proc. of 8th International Carbon Dioxide Conference.-2009.-P.T2-098.
54. Glushkov A.V., Khetselius O., Svinarenko A.A., Lovett L., Energy approach to nuclei and atoms in a strong laser field: Stark effect and multiphoton resonances // Quantum Theory: Reconsideration of Foundations. AIP Conf.Proc.-2010.-Vol.1232.-P.228-234.
55. 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.
56. 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.
57. 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.-525-541.
58. 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.
59. Glushkov A.V., Khetselius O., Svinarenko 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. Chemistry and Physics, Eds. P.Hoggan, E.Brandas, J.Maruani, G. Delgado-Barrio, P.Piecuch (Springer).-2012.-Vol.22.-P.51-68.
60. Glushkov A.V., Relativistic Quantum Theory. Quantum mechanics of Atomic Systems.-Odessa: Astroprint, 2008. -700P.
61. Glushkov A.V., Khetselius O.Yu., Prepelitsa G., 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 International Geometry Center".-2013.-Vol.6, N1.-P.43-48.
62. 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.
63. Malinovskaya S., Glushkov A., Khetselius O., Lopatkin Yu., Loboda A.V., Svinarenko 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,N2.-P.288-296.
64. Malinovskaya S.V., Glushkov A.V., Khetselius O.Yu., Svinarenko A.A., Mischenko E.V., Florko T.A., Optimized 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.
65. Glushkov A.V., Relativistic and correlation effects in spectra of atomic systems.-Odessa: Astroprint.-2006.-400P.
66. Glushkov A.V., Khetselius O.Y., Malinovskaya S.V., Spectroscopy of cooperative laser-electron nuclear effects in multiatomic molecules// Molec. Physics. (UK).-2008.-Vol.106, N9-10.-P.1257-1260.
67. 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. Proc.-2010.-Vol.1290.-P. 263-268.
68. 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.
69. Glushkov A V, Ivanov L N, DC Strong Field Stark Effect for Non-hydrogenic Atoms: Consistent Quantum Mechanical Approach // Journal of Physics B: Atomic, Molecular and Optical Phys.-1993.-Vol.26,N14.-P.L379 – L386.
70. 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.
71. 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.-P.1717-1727.
72. 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. Quant. Chem.-2009.-Vol.109,N14.-P.3473-3481.
73. Glushkov A.V., Khetselius O.Yu., Gurnitskaya E.P., Loboda A.V., Florko T.A., Sukharev D.E., Lovett L., Gauge-Invariant QED Perturbation Theory Approach to Calculating Nuclear Electric Quadrupole Moments, Hyperfine Structure Constants for Heavy Atoms and Ions//Frontiers in Quantum Systems in Chemistry and Physics (Springer), 2008.-Vol.18.-P.507-524.
74. Khetselius O Yu, Relativistic calculation of the hyperfine structure parameters for heavy elements and laser detection of the heavy isotopes// Phys. Scripta.-2009.-Vol.T135.-P.014023.
75. 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 Theoretical Chemistry and Physics (Springer, Dordrecht).-2012-Vol.26.-P.217-229.
76. Buyadzhi V V , Glushkov A V, Spectroscopy of atom and nucleus in a strong laser field: Stark effect and multiphoton resonances//Photoelectronics.-2014.-Issue 23.-P.38-43
77. 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. Ed. G.Fazio, F.Hanappe, Singapore : World Scientific.-2003.-P.126-132.

UDC 539.182

I. N. Serga, O. Yu. Khetselius, L. A. Vitavetskaya, A. N. Bystryantseva

RELATIVISTIC THEORY OF SPECTRA OF PIONIC ATOMIC SYSTEM ^{208}Pb WITH ACCOUNT OF STRONG PION-NUCLEAR INTERACTION EFFECTS

Abstract. It is presented a consistent relativistic theory of spectra of the pionic atoms on the basis of the Klein-Gordon-Fock with a generalized radiation and strong pion-nuclear potentials. It is applied to calculation of the energy and spectral parameters for pionic atoms of the ^{208}Pb with accounting for the radiation (vacuum polarization), nuclear (finite size of a nucleus) and the strong pion-nuclear interaction corrections. The measured values of the Berkley, CERN and Virginia laboratories and alternative data based on other versions of the Klein-Gordon-Fock theories with taking into account for a finite size of the nucleus in the model uniformly charged sphere and the standard Uehling-Serber radiation correction and optical atomic theory are listed too. There are listed new data on shift and broadening of the 4f level in ^{208}Pb due to the strong pion-nuclear intetraction.

Key words: strong interaction, pionic atom ^{208}Pb, relativistic theory

УДК 539.182

И. Н. Серга, О. Ю. Хецелиус, Л. А. Витавецкая, А. Н. Быстрянцева

РЕЛЯТИВИСТСКАЯ ТЕОРИЯ СПЕКТРОВ ПИОННЫХ АТОМНЫХ СИСТЕМ ^{208}Pb С УЧЕТОМ ЭФФЕКТОВ СИЛЬНОГО ПИОН-ЯДЕРНОГО ВЗАИМОДЕЙСТВИЯ

Резюме. Представлена последовательная релятивистская теория спектров пионных атомов на основе уравнения Клейна-Гордона-Фока с обобщенными радиационным и сильным пион-ядерным потенциалом. Выполнен расчет энергетических и спектральных параметров для пионного атома ^{208}Pb, с учетом радиационных (поляризация вакуума), ядерных (конечный размер ядра) эффектов и поправки на сильное пион-нуклонное взаимодействие. Также для сравнения

представлены данные измерений в лабораториях Berkley, ЦЕРН и Вирджиния и теоретические результаты, полученные на основе альтернативных теорий Клейна-Гордона-Фока с учетом конечного размера ядра в модели равномерно заряженной сферы и стандартной Юлинг-Сербер поправки. Представлены новые данные по сдвигу и уширению 4f уровня в атоме ^{208}Pb благодаря сильному пион-ядерному взаимодействию.

Ключевые слова: сильное взаимодействие, пионный атом ^{208}Pb, релятивистская теория

УДК 539.182

І. М. Сєрга, О. Ю. Хецеліус, Л. А. Вітавецька, А. М. Бистрянцева

РЕЛЯТИВІСТСЬКА ТЕОРІЯ СПЕКТРІВ ПІОННИХ АТОМНИХ СИСТЕМ ^{208}Pb З УРАХУВАННЯМ ЕФЕКТІВ СИЛЬНОЇ ПІОН-ЯДЕРНОЇ ВЗАЄМОДІЇ

Резюме. Представлена послідовна релятивістська теорія спектрів півоній атомів на основі рівняння Клейна-Гордона-Фока з узагальненими радіаційним і сильним півонія-ядерним потенціалом. Виконано розрахунок енергетичних і спектральних параметрів для піоного атома ^{208}Pb з урахуванням радіаційних (поляризація вакууму), ядерних (кінцевий розмір ядра) ефектів та поправки на сильну піон-нуклонну взаємодію. Також для порівняння представлені дані вимірювань в лабораторіях Berkley, ЦЕРН і Вірджинія і теоретичні результати, отримані на основі альтернативних теорій Клейна-Гордона-Фока з урахуванням кінцевого розміру ядра в моделі рівномірно зарядженої сфери і стандартної Юлінг-Сербер поправки. Представлені нові данні щодо зсуву та уширення 4f рівня в атомі ^{208}Pb завдяки сильній піон-ядерній взаємодії

Ключові слова: сильна взаємодія, піонний атом ^{208}Pb, релятивістська теорія

UDC 539.186

A. A. Kuznetsova[1], Yu. V. Dubrovskaya[2], A. V. Glushkov[2], Ya. I. Lepikh[3]

[1]Odessa National Maritime Academy, Didrikhsona str. 4, Odessa, 65001
[2]Odessa State Environmental University, 15, Lvovskaya str., Odessa, 65016
[3]I. I. Mechnikov's Odessa National University, Dvoryanskaya str., 2, Odessa, 65028
E-mail: kuznetsovaa232@gmail.com

ADVANCED GREEN'S FUNCTIONS AND DENSITY FUNCTIONAL APPROACH TO VIBRATIONAL STRUCTURE IN THE PHOTOELECTRON SPECTRA OF DIATOMIC MOLECULE

The advanced combined theoretical approach to vibrational structure in photoelectron spectra of diatomic molecules, which is based on the density functional theory (DFT) and the Green's-functions approach, is used for quantitative treating the diatomic photoelectron spectra. The density of states, which describe the vibrational structure in photoelectron spectra, is defined with the use of combined DFT-Green's-functions approach and is well approximated by using only the first order coupling constants in the one-particle approximation. Using the DFT theory leads to significant simplification of the calculation.

1. Introduction

The Green's method is very well known in a quantum theory of field, quantum theory of solids. Naturally, an attractive idea was to use it in the molecular theory. Regarding a problem of description of the vibrational structure in photoelectron spectra of molecules, it is easily understand that this approach has great perspective (c.f.[1-51]). One could note that the experimental photoelectron (PE) spectra usually show a pronounced vibrational structure. Usually the electronic Green's function is defined for fixed position of the nuclei. As result, only vertical ionization potentials (V.I.P.'s) can be calculated [11,2,11,12]. The cited method, however, requires as input data the geometries, frequencies, and potential functions of the initial and final states. Since in most cases at least a part of these data are unavailable, the calculations have been carried out with the objective of determining the missing data by comparison with experiment. Naturally, the Franck-Condon factors are functions of the derivatives of the difference between the potential curves of the initial and final states with respect to the normal coordinates. To avoid the difficulty and to gain additional information about the ionization process, the Green's functions approach has been extended to include the vibrational effects in the photoelectron spectra. Nevertheless, there are well known great difficulties of the correct interpretation of the photoelectron spectra for any molecules.

Here we present the advanced combined theoretical approach to vibrational structure in photoelectron spectra of diatomic molecules and use it for effective quantitative treating the diatomics photoelectron spectra. The advanced approach is based on the Green's function method (Cederbaum-Domske version) [11,12], Fermi-liquid DFT formalism [1-8] and use of the novel effective density functionals (see also [13-16]). As usually (see Refs. [2,4,11]), the density of states, which describe the vibrational structure in molecular photoelectron spectra, is calculated with the help of combined DFT-Green's-functions approach. In addition to exact solution of one-bode problem different approaches to calculate reorganization and many-body effects are presented. The density of states is well approximated by using only the first order coupling constants in the one-particle approximation. It is important that the calculational procedure is significantly simplified with using the quasiparticle DFT formalism. Thus quite simple method becomes a powerful

tool in interpreting the vibrational structure of photoelectron spectra for different molecular systems.

2. Method: Density of states in one-body and many-body solution

As usually (see details in refs. [1-12]), the quantity which contains the information about the ionization potentials (I.P.) and molecular vibrational structure due to quick ionization is the density of occupied states:

$$N_k(\epsilon) = (1/2\pi\hbar)\int dt e^{i\hbar^{-1}\epsilon t}\langle\psi_0|a_k^t(0)a_k(t)|\psi_0\rangle, \quad (1)$$

where $|\Psi_0\rangle$ is the exact ground state wave function of the reference molecule and $a_k(t)$ is an electron destruction operator, both in the Heisenberg picture. For particle attachment the quantity of interest is the density of unoccupied states:

$$N_k(\epsilon) = (1/2\pi\hbar)\int dt e^{i\hbar^{-1}\epsilon t}\langle\psi_0|a_k(t)a_k^t(0)|\psi_0\rangle \quad (2)$$

Usually in order to calculate the value (1) states for photon absorption one should express the Hamiltonian of the molecule in the second quantization formalism. The Hamiltonian is as follows:

$$H = T_E(\partial/\partial x) + T_N(\partial/\partial X) + U_E(x) + U_N(X) + U_{EN}(x,X) \quad (3)$$

where T_E and T_N are the kinetic energy operators for electrons and nuclei, and U represents the interaction; U_E represents the Coulomb interaction between electrons, etc; x (X) denotes electron (nuclear) coordinates. As usually, introducing a field operator $\Psi(R,\theta,x) = \sum_i \phi_i(x,R,\theta)a_i(R,\theta)$ with the Hartree-Fock (HF) one–particle functions ϕ_i ($\epsilon_i(R)$ are the one-particle HF energies and f denotes the set of orbitals occupied in the HF ground state; R_0 is the equilibrium geometry on the HF level) and dimensionless normal coordinates Q_s one can write the standard Hamiltonian as follows [2,11]:

$$H = H_E + H_N + H_{EN}^{(1)} + H_{EN}^{(2)}, \quad (4)$$

$$H_E = \sum_i^{\epsilon} V_i(R_0)a_i^t a_i + \frac{1}{2}\sum V_{ijkl}(R_0)a_i^t a_j^t a_l a_k - \sum_{i,j}\sum_{k\in f}[V_{ikjk}(R_0) - V_{ikkj}(R_0)]a_i^t a_j,$$

$$H_N = \hbar\sum_{s=1}^{M}\omega_s(b_s^t b_s + \frac{1}{2}),$$

$$H_{EN}^{(1)} = 2^{-1/2}\sum_{s=1}^{M}\left(\frac{\partial_i V_i}{\partial Q_s}\right)_0 (b_s + b_s^t)[a_i^t a_i - n_i] + \frac{1}{4}\sum_i\sum_{s,s'=1}^{M}\left(\frac{\partial^2 V_i}{\partial Q_s \partial Q_{s'}}\right)_0 (b_s + b_s^t)(b_{s'} + b_{s'}^t)[a_i^t a_i -$$

$$H_{EN}^{(2)} = 2^{-3/2}\sum\sum_{s=1}^{M}\left(\frac{\partial V_{ijkl}}{\partial Q_s}\right)_0 (b_s + b_s^t)[\delta v_1 a_i^t a_j^t a_k + \delta v_2 a_l a_k a_i^t a_j^t + 2\delta v_3 a_j^t a_k a_l a_i^t] +$$

$$+ \frac{1}{8}\sum\sum_{s,s'=1}^{M}\left(\frac{\partial^2 V_{ijkl}}{\partial Q_s \partial Q_{s''}}\right)_0 (b_s + b_s^t)(b_{s'} + b_{s'}^t \cdot [\delta v_1 a_i^t a_j^t a_k + \delta v_2 a_l a_k a_i^t a_j^t + 2\delta v_3 a_j^t a_k a_l a_i^t],$$

with n_i=1 (0), $i\epsilon f$ ($i\epsilon f$), $\delta\sigma_f$=1 (0) , $(ijkl)\epsilon\sigma_{f...}$ where the index set v_1 means that at least ϕ_k and ϕ_l or ϕ_i and ϕ_j are unoccupied, v_2 that at most one of the orbitals is unoccupied, and v_3 that ϕ_k and ϕ_j or ϕ_l and ϕ_j are unoccupied. Here for simplicity all terms leading to anharmonicities are neglected. The ω_s are the HF frequencies; b_s, b_s^t are destruction and creation operators for vibrational quanta as

$$Q_s = (1/\sqrt{2})(b_s + b_s^t)$$
$$\partial/\partial Q_s = (1/\sqrt{2})(b_s - b_s^t). \quad (5)$$

The interpretation of the above Hamiltonian and an exact solution of the one-body HF problem is given in refs. [1,2,11,12]. The HF-single-particle component H_0 of the Hamiltonian (4) is as follows:

$$H_0 = \sum_i \varepsilon^o{}_i(R_0) a_i^t a_i + \sum_{s=1}^{M} \hbar\omega_s (b_s^t b_s + \frac{1}{2}) +$$
$$\sum_{s=1}^{M} \sum_i 2^{-1/2} \left(\frac{\partial^o V_i}{\partial Q_s} \right) [a_i^t a_i - n_i] (b_s + b_s^t)_0 +$$
$$+ \sum_{s,s'=1} \sum_i \frac{1}{4} \left(\frac{\partial^{2o} V_i}{\partial Q_s \partial Q_{s'}} \right)_0 [a_i^t a_i - n_i] \cdot$$
$$\cdot (b_s + b_s^t)(b_{s'} + b_{s'}^t) \qquad (6)$$

Correspondingly in the one-particle picture the density of occupied states is given by

$$N_k^0(\omega) = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} dt e^{i\hbar^{-1}(\omega - \varepsilon_k)t} \langle 0 | e^{\pm i\hbar^{-1}\tilde{H}_0 t} | 0 \rangle, \qquad (7)$$

$$\tilde{H}_0 = \sum_{s=1}^{M} \hbar\omega_s b_s^t b_s + \sum_{s=1}^{M} g_s^k (b_s + b_s^t) +$$
$$+ \sum_{s,s'=1}^{M} \gamma_{ss'}^k (b_s + b_s^t)(b_{s'} + b_{s'}^t) \qquad (8)$$

$$g_s^i = \pm \frac{1}{\sqrt{2}} \left(\frac{\partial^o{}_i}{\partial Q_s} \right)_0, \quad \gamma_{ss'}^i = \pm \frac{1}{4} \left(\frac{\partial^{2o}{}_i}{\partial Q_s \partial Q_{s'}} \right)_0 . \qquad (9)$$

Introducing new operators

$$c_s = \sum_{l=1}^{M} (\lambda_1^s b_l + \lambda_2^s b_l^t) \qquad (10)$$

with real coefficients λ_1^s, λ_2^s, defined in such a way that $\tilde{H}_0$ in new operators is

$$\tilde{H}_0 = \sum_{s=1}^{M} \hbar\hat{\omega}_s c_s^t c_s + \sum_{s=1}^{M} \hat{g}_s (c_s + c_s^t) + k. \qquad (11)$$

eq. (7) is as follows:

$$N_k^0(\omega) = \sum_{n_1 \cdots n_M} | \langle \hat{n} | U | 0 \rangle |^2 \delta(\omega - \omega_k \pm \Delta\omega_k \pm n \cdot \hbar\hat{\omega}) \qquad (12)$$

where δ function in (12) naturally contains the information about adiabatic ionization potential and the spacing of the vibrational peaks; $| \langle \hat{n} | U | 0 \rangle |^2$ is the well-known Franck-Condon factor. In a diagrammatic method to get function $N_k(\omega)$ one should calculate the GF $G_{kk'}(\omega)$ first [1,2,11,12]:

$$G_{kk'}(\omega) = -i\hbar^{-1} \int_{-\infty}^{\infty} dt e^{i\hbar^{-1}\eta} \langle \psi_0 | \hat{O}\{ a_k(t) a_{k'}^t(0) \} | \psi_0 \rangle \qquad (13)$$

and the function $N_k(\omega)$ can be found from the relation

$$\pi N_k(\omega) = a \operatorname{Im} G_{kk}(\omega - i\eta), \; a = -sign \omega_k . \qquad (14)$$

Choosing the unperturbed Hamiltonian H_0 to be $H_0 = \sum \omega_i a_i^t a_i + H_N$ one finds the GF. In the known approximation GF is as follows:

$$G_{kk'}^{\omega}(t) = \pm\delta_{kk'} i \exp[-i\eta^{-1}(\varepsilon_k \mp \Delta\varepsilon)t] \cdot$$
$$\cdot \sum_n | \langle \hat{n}_k | U_k | 0 \rangle |^2 \exp(\pm i\eta_k \cdot \hat{\omega}_k t) \qquad , \qquad (15)$$

The direct method for calculation of $N_k(\in)$ as the imaginary part of the GF includes a definition of the vertical I.P. (V.I.P.s) of the reference molecule and then of $N_k(\in)$. The zeros of the functions

$$D_k(\in) = \in - [\in^{\omega} + \Sigma(\in)]_k , \qquad (16)$$

where $(\in^{\omega} + \Sigma)_k$ denotes the k-th eigenvalue of the diagonal matrix of the one-particle energies added to matrix of the self-energy part, are the negative V. I. P. 's for a given geometry. One can write [2,11,12]:

$$(V.I.P.)_k = -(\in_k + F_k)$$

$$F_k = \Sigma_{kk} (-(V.I.P.)_k) \approx \frac{1}{1 - \partial\Sigma_{kk}(\in_k)/\partial_{\in}} \Sigma_{kk}(\in_k) \quad . \qquad (17)$$

Expanding the ionic energy E_k^{N-1} about the equilibrium geometry of the reference molecule in a power series of the normal coordinates of this molecule leads to a set of linear equations in the unknown normal coordinate shifts δQ_S, and new coupling constants are then:

$$g_1 = \pm(1/\sqrt{2}) [\partial(\in_k + F_k)/\partial Q_l]_0 \qquad (18)$$
$$\gamma_{ll'} = \pm \left(\frac{1}{4} \right) [\partial^2(\in_k + F_k)/\partial Q_l / \partial Q_{l'}]_0$$

The coupling constants g_l and $y_{ll'}$ are calculated by the well-known perturbation expansion of the

self-energy part using the Hamiltonian H_{EN} of Eq. (3). In second order one obtains:

$$\sum\nolimits_{lk}^{(2)}(\in)=\sum_{\substack{i,j\\ s\notin F}}\frac{(V_{ksij}-V_{ksji})V_{ksij}}{\in+\in_s-\in_i-\in_j}+\sum_{\substack{i,j\\ s\notin F}}\frac{(V_{ksij}-V_{ksji})V_{ksij}}{\in+\in_s-\in_i-\in_j} \tag{19}$$

and the coupling constant g_l are written as

$$g_l\approx\pm\frac{1}{\sqrt{2}}\frac{\partial\in_k}{\partial Q_l}\frac{1+q_k(\partial/\partial\in)\sum_k[-(V.I.P.)_k]}{1-(\partial/\partial\in)\sum_k[-(V.I.P.)_k]},$$

$$q_k=A/B$$

$$A=\sum\frac{(V_{ksij}-V_{ksji})^2}{[-(V.I.P.)_k+\in_s-\in_i-\in_j]^2}\bullet$$

$$\bullet\left[\frac{\partial\in_s}{\partial Q_l}-\frac{\partial\in_i}{\partial Q_l}-\frac{\partial\in_j}{\partial Q_l}\right]$$

$$B=\frac{\partial\in_k}{\partial Q_l}\sum\frac{(V_{ksij}-V_{ksji})^2}{[-(V.I.P.)_k+\in_s-\in_i-\in_j]^2} \tag{20}$$

It is suitable to use further the pole strength of the corresponding GF:

$$\rho_k=\left\{1-\frac{\partial}{\partial\in}\sum\nolimits_k[-(V.I.P)_k]\right\}^{-1};1\geq\rho_k\geq 0,$$

$$g_l\approx g_l^0[\rho_k+q_k(\rho_k-1)],$$

$$g_l^0=\pm 2^{-1/2}\partial\in_k/\partial Q_l \tag{21}$$

Below we give the DFT definition of the pole strength corresponding to V. I. P.'s and confirm the earlier data [11-15]: $p_k\approx 0,8$-0,95. The coupling constant is:

$$\gamma_{lk}=\gamma_l^0\left(\frac{g_l}{g_l^0}\right)+\frac{1}{4}\sqrt{2}g_l^0\frac{\partial}{\partial Q_l}\left(\frac{g_l}{g_l^0}\right) \tag{22}$$

3. Fermi-liquid quasiparticle density functional theory

Further we consider the quasiparticle Fermi-liquid version of the DFT, following to refs. [1-3,8,17]. The master equations can be obtained on the basis of variational principle, if we start from a Lagrangian of a molecule L_q. It should be defined as a functional of quasiparticle densities:

$$\nu_0(r)=\sum_\lambda n_\lambda|\Phi_\lambda(r)|^2,$$

$$\nu_1(r)=\sum_\lambda n_\lambda|\nabla\Phi_\lambda(r)|^2, \tag{23}$$

$$\nu_2(r)=\sum_\lambda n_\lambda[\Phi_\lambda^*\Phi_\lambda-\Phi_\lambda^*\Phi_\lambda]$$

The densities ν_0 and ν_1 are similar to the HF electron density and kinetical energy density correspondingly; the density ν_2 has no an analog in the HF or DFT theory and appears as result of account for the energy dependence of the mass operator Σ. A Lagrangian L_q can be written as a sum of a free Lagrangian and Lagrangian of interaction: $L_q=L_q^0+L_q^{int}$, where a free Lagrangian L_q^0 has a standard form:

$$L_q^0=\int d\sum_\lambda n_\lambda\Phi_\lambda^*(i\partial/\partial t-\varepsilon_p)\Phi_\lambda, \tag{24}$$

The interaction Lagrangian is defined in the form, which is characteristic for a standard DFT (as a sum of the Coulomb and exchange-correlation terms), however, it takes into account for the energy dependence of a mass operator Σ :

$$L_q^{\text{int}}=L_K-\frac{1}{2}\sum_{i,k=0}^{2}\int\beta_{ik}F(r_1,r_2)\nu_i(r_1)\nu_k(r_2)dr_1dr_2 \tag{25}$$

where β_{ik} are some constants (look below), F is an effective potential of the exchange-correlation interaction. The Coulomb interaction part L_K looks as follows:

$$L_K=-\frac{1}{2}\int[1-\sum\nolimits_2(r_1)]\nu_0(r_1)[1-$$
$$-\sum\nolimits_2(r_2)]\nu_0(r_2)/|r_1-r_2|dr_1dr_2 \tag{26}$$

where $\Sigma_2=\partial\Sigma/\partial\varepsilon$. In the local density approximation the potential F can be expressed through the exchange-correlation pseudopotential V_{xc} as follows:

$$F(r_1,r_2)=\delta V_{xc}/\delta\nu_0\cdot\delta(r_1-r_2). \tag{27}$$

Further, one can get the following expressions for $\Sigma_i=-\delta L_q^{\text{int}}/\delta\nu_i$:, in particular:

$$\Sigma_1 = \beta_{01}\delta V_{XC}/\delta\nu_0\cdot\nu_0 + \beta_{12}\delta V_{XC}/\delta\nu_0\cdot\nu_2 + \\ + \beta_{11}\delta V_{XC}/\delta\nu_0\cdot\nu_1$$

$$\Sigma_2 = \beta_{02}\delta V_{XC}/\delta\nu_0\cdot\nu_0 + \beta_{12}\delta V_{XC}/\delta\nu_0\cdot\nu_1 + \\ + \beta_{22}\delta V_{XC}/\delta\nu_0\cdot\nu_2 \qquad (28)$$

Here V_K is the Coulomb term, Σ_0^{α} is the exchange term. Using the known canonical relationship, one can derive the quasiparticle Hamiltonian, which is corresponding to L_q .Further constants β_{ik} should be defined. In some degree they have the same essence as the similar constants in the well-known Landau Fermi-liquid theory and the Migdal finite Fermi-systems theory. Regarding universality of β_{ik},, indeed, as we know now, the total universality of the constants in the last theories is absent, though a range of its changing is quite small [2,17]. The value of β_{00} is dependent on definition of V_{xc}. If as V_{xc} it is used one of the DFT exchange-correlation potentials from, then without losing a community of statement, β_{00}=1. The constant β_{02} can be in principle calculated by analytical way, but it is very useful to remember its connection with a spectroscopic factor F_{sp} of the system [18]:

$$F_{sp} = \left\{1 - \frac{\partial}{\partial \in}\sum_k \left[-(V.I.P)_k\right]\right\} \qquad (29)$$

The terms $\partial\sum/\partial\varepsilon$ and $\sum_2$ is directly linked [2,17]. In the terms of the Green function method expression (7) is in fact corresponding to the pole strength of the Green's function [2]. The new element of an approach can be connected with using the DFT correlation functional of the Lee-Yang-Parr (LYP) (look details in ref. [13-16]).

3. Results and conclusions

As illustration, we choose the diatomic molecule of N_2 for application of the combined Green's function method and quasiparticle DFT approach. The nitrogen molecule has been naturally discussed in many papers. The valence V. I. P. 's of N_2 have been calculated [1,13,14,24] by the method of Green's functions and therefore the pole strengths p_k are known and the mean values q_k can be estimated. It should be reminded that the N_2 molecule is the classical example where the known Koopmans' theorem even fails in reproducing the sequence of the V. I. P. 's in the PE spectrum. From the HF calculation of Cade *et al.*[24] one finds that including reorganization the V. I. P. 's assigned by σ_g and σ_u improve while for π V. I. P. the good agreement between the Koopmans value and the experimental one is lost, leading to the same sequence as given by Koopmans' theorem. In Table 1 the experimental V. I. P. 's (a), the one-particle HF energies (b), the V. I. P. 's calculated by Koopmans' theorem plus the contribution of reorganization (c), the V. I. P. 's calculated with Green's functions method (d), the combined Green functions and DFT approach (e), the similar our results (f).

Table 1

The experimental and calculated V. I. P.'s (in eV) of N_2. R_k is the contribution of reorganization; p_k stands for pole strength.

Orbital	Exptl[a] V.I.P.'s	$-\epsilon_k^b$	$-(\epsilon_k + R_k)^c$
$3\sigma_g$	15,60	17,36	16,01
$1\pi_u$	16,98	17,10	15,67
$2\sigma_u$	18,78	20,92	19,93
Orbital	Calc[d] V.I.P.'s	Calc[e] V.I.P.'s	Calc[f] V. I. P. ' ρ_k^e
$3\sigma_g$	15,50	15,52	15,58
$1\pi_u$	16,83	16,85	16,96
$2\sigma_u$	18,59	18,63	18,76

The important point of all consideration is connected the principal possibility to reproduce diatomic spectra by applying a one-particle theory with account of the correlation and reorganization effects. The combined theoretical approach, which is based on the quasiparticle DFT with using

correct DF and the Green's-functions approach can be prospectively used for quantitative treating the diatomic photoelectron spectra. It is very important that the computational complexity of the combined approach is significantly lower in comparison with original version of the Green's-functions method.

References

1. Glushkov A.V., New approach to theoretical definition of ionization potentials for molecules on the basis of Green's function method//Journ.of Phys. Chem.-1992.-Vol.66.-P.2671-2677.
2. Glushkov A.V., Relativistic quantum theory. Quantum mechanics of atomic systems.-Odessa: Astroprint, 2008.-700P.
3. Glushkov A.V., The Green's functions and density functional approach to vibrational structure in the photoelectron spectra of molecules: Review of method// Photoelectronics.-2014.-Vol.23.-P.54-72.
4. Glushkov A.V., Lepikh Ya.I., Fedchuk A.P., Loboda A.V., The Green's functions and density functional approach to vibrational structure in the photoelectron spectra of molecules//Photoelectronics.-2009.-N18.-P.119-127.
5. Svinarenko A.A., Fedchuk A.P., Glushkov A.V.,Lepikh Ya.I., Loboda A.V., Lopatkin Yu.M., The Green's functions and density functional approach to vibrational structure in the photoelectron spectra of carbon oxide molecule//Photoelectronics.-2010.-N19.-P.115-120.
6. Glushkov A.V., Fedchuk A.P., Kondratenko P.A., Lepikh Ya.I., Lopatkin Yu.M., Svinarenko A.A., The Green's functions and density functional approach to vibrational structure in the photoelectron spectra: Molecules of CH, HF//Photoelectronics.-2011.-Vol.20.-P.58-62.
7. Glushkov A.., Koltzova N., Effective account of polarization effects in calculation of oscillator strengths and energies for atoms and molecules by method of equations of motion// Opt. Spectr. -1994.- Vol. 76,№6.-P.885-890.
8. Glushkov A.V., Quasiparticle approach in the density functional theory under finte temperatures and dynamics of effective Bose -condensate // Ukr. Phys. Journ.- 1993.-Vol. 38, №8.-P.152-157.
9. Ponomarenko E.L., Kuznetsova A.A., Dubrovskaya Yu.V., Bakunina (Mischenko) E.V., Energy and spectroscopic parameters of diatomics within generalized equation of motion method// Photoelectronics.-2016.-Vol.25.-P.114-118.
10. Mischenko E.V., An effective account of correlation in calculation of excited states energies for molecules by equation of motion method: O_3//Photoelectronics.-2007.-N16.-P.123-125.
11. Köppel H., Domcke W., Cederbaum L.S., Green's function method in quantum chemistry// Adv. Chem. Phys.-1994.-Vol.57.-P.59-132.
12. Cederbaum L.S., Domcke W., On vibrational structure of photoelectron spectra by the Green's functions method// J.Chem. Phys.-1984.-Vol.60.-P.2878-2896.
13. Zangwill A.,Soven P.J. Density-functional approach to local field effects in finite systems. Photo-absorption in rare gases // Phys.Rev.A.-1990.-Vol.21,N5-P.1561-1572.
14. Kobayashi K., Kurita N., Kumahora H., Kuzatami T. Bond-energy calculations of Cu , Ag, CuAg with the generalized gradient approximation// Phys. Rev.A.-1991.-Vol.43.-P.5810-5813.
15. Lagowscki J.B., Vosko S.H. Analysis of local and gradient- correction correlation energy functionals using electron removal energies// J. Phys.B: At. Mol. Opt. Phys.-1998.-Vol.21,N1-P.203-208.
16. Guo Y., Whitehead M.A. Effect of the correlation correction on the ionization potential and electron affinity in atoms// Phys.Rev.A-1999.-Vol.39,N1.-P.28-34.

17. Glushkov A.V., An universal quasiparticle energy functional in a density functional theory for relativistic atom// Optics and Spectr.-1999.-Vol.66,N1-P.31-36.
18. Glushkov A.V., Relativistic and correlation effects in spectra of atomic systems.-Odessa: Astroprint.-2006.-400P.
19. Glushkov A.V., Atom in electromagnetic field.-Kiev: KNT, 2005.-450P.
20. Khetselius O.Yu., Hyperfine structure of atomic spectra.-Odessa: Astroprint, 2008.-210P.
21. Glushkov A.V., Khetselius O.Y., Malinovskaya S.V., Spectroscopy of cooperative laser-electron nuclear effects in multiatomic molecules// Molec. Phys.-2008. -Vol.106.-N9-10.-P.1257-1260.
22. 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.-525-541.
23. Glushkov A.V., Khetselius O.Yu., Svinarenko A.A., Prepelitsa G.P. , Shakhman A., Spectroscopy of cooperative laser-electron nuclear processes in diatomic and multiatomic molecules//Spectral Lines Shape (AIP, USA).-2010.-Vol.16.-P.269-273.
24. Glushkov A.V., Kondratenko P.A., Buyadzhi V., Kvasikova A.S., Shakhman A., Sakun T., Spectroscopy of cooperative laser electron-γ-nuclear processes in polyatomic molecules// Journal of Physics: C Series (IOP, London, UK).-2014.-Vol.548.-P. 012025 (5p.).
25. Glushkov A.V., Kondratenko P.A., Lopatkin Yu., Buyadzhi V., Kvasikova A., Spectroscopy of cooperative laser electron- γ -nuclear processes in diatomics and multiatomic molecules // Photoelectronics.-2014.-Vol.23.-P.142-146.
26. 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.Brändas, G.Delgado-Barrio (Springer).-2015-Vol.29.-P.55-76.
27. 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.217-229.
28. 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.
29. Khetselius O., Spectroscopy of cooperative electron-gamma-nuclear processes in heavy atoms: NEET effect// J. Phys.: Conf. Ser.-2012.- Vol.397.-P.012012
30. 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.
31. 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.
32. Glushkov A.V., Khetselius O., Svinarenko 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.

33. Glushkov A.V., Khetselius O.Yu., Prepelitsa G., 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 International Geometry Center".-2013.-Vol.6, N1.-P.43-48.
34. 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.
35. Malinovskaya S.V., Glushkov A.V., Khetselius O.Yu., Lopatkin Yu., Loboda A., Svinarenko 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,N2.-P.288-296.
36. Malinovskaya S.V., Glushkov A.V., Khetselius O.Yu., Svinarenko A.A., Mischenko E.V., Florko T.A., Optimized 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.
37. Glushkov A.V., Khetselius O.Yu., Svinarenko A., Prepelitsa G., Mischenko E., 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.
38. 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.
39. Khetselius O.Yu., Hyperfine structure of radium// Photoelectronics.-2005.-N14.-P.83-85.
40. 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, F.Hanappe, Singapore: World Scientific.-2003.-P.242-250.
41. Glushkov A.V., Lovett L., Khetselius O., Gurnitskaya E., Dubrovskaya Yu., Loboda A., 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.
42. Glushkov A., Malinovskaya S., Sukharev D., Khetselius O.Yu., Loboda A., 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.J. Quant. Chem.-2009.- Vol. 109.-N8.-P.1717-1727.
43. 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.
44. 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.
45. 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.
46. Glushkov A.V., Effective quasi-particle valence hamiltonian of molecules in the comprehensive semi-empirical theory// Sov. J. Struct. Chem.-1998.-Vol.29,N4.-P.3-9.
47. Khetselius O.Yu., Quantum Geometry: New approach to quantization of the quasistationary states of Dirac equation for super heavy ion and calculating hyper fine structure parameters// Proc. Int. Geometry Center.-2012.-Vol.5,№ 3-4.-P.39-45.
48. 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.
49. Gedasimov V N, Zelenkov A G, Kulakov V M et al 1994 *JETP.* **86** 1169; Soldatov A A 1983 Preprint of I.V.Kurchatov Institute for Atomic Energy IAE-3916, Moscow
50. 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.
51. 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. J. Quantum Chem.-2009.-Vol.109, N14.-P.3473-3481.

This article has been received in May 2017

UDC 539.186

A. A. Kuznetsova, Yu. V. Dubrovskaya, A. V. Glushkov, Ya. I Lepikh

ADVANCED GREEN'S FUNCTIONS AND DENSITY FUNCTIONAL APPROACH TO VIBRATIONAL STRUCTURE IN THE PHOTOELECTRON SPECTRA OF DIATOMIC MOLECULE

Summary

The advanced combined theoretical approach to vibrational structure in photoelectron spectra of molecules, which is based on the density functional theory (DFT) and the Green's-functions (GF) approach, is used for quantitative treating the diatomics photoelectron spectra. The density of states, which describe the vibrational structure in photoelectron spectra, is defined with the use of combined 'density functional-Green's functions' approach and is well approximated by using only the first order coupling constants in the one-particle approximation. Using the DFT theory leads to significant simplification of the molecular calculations.

Key words: photoelectron spectra of molecules, Green's functions, density functional theory

УДК 539.186

А. А. Кузнецова, Ю. В. Дубровская, А. В. Глушков, Я. И. Лепих

ОБОБЩЕННЫЙ МЕТОД ФУНКЦИЙ ГРИНА И ФУНКЦИОНАЛА ПЛОТНОСТИ В ОПРЕДЕЛЕНИИ КОЛЕБАТЕЛЬНОЙ СТРУКТУРЫ ФОТОЭЛЕКТРОННОГО СПЕКТРА ДВУХАТОМНЫХ МОЛЕКУЛ

Резюме

Усовершенствованный комбинированный теоретический метод описания вибрационной структуры для фотоэлектронных спектров молекул, основанный на методе функций Грина и теории функционала плотности, применен к количественному описанию фотоэлектронного спектра двухатомных молекул. Плотность состояний, которые описывают колебательную структуру в фотоэлектронных спектрах, определяется с использованием комбинированного подхода (метод функционала плотности и функций Грина) и хорошо аппроксимируется с использованием только первого порядка констант связи в одноквазичастичном приближении. Использование теории функционала плотности приводит к значительному упрощению молекулярных расчетов.

Ключевые слова: фотоэлектронный спектр молекул, метод функций Грина, теория функционала плотности

УДК 539.186

Г. О. Кузнецова, Ю. В. Дубровська, О. В. Глушков, Я. І. Лепіх

УДОСКОНАЛЕНИЙ МЕТОД ФУНКЦІЙ ГРІНА І ФУНКЦІОНАЛУ ГУСТИНИ У ВИЗНАЧЕННІ ВІБРАЦІЙНОЇ СТРУКТУРИ ФОТОЕЛЕКТРОННОГО СПЕКТРУ ДВОАТОМНИХ МОЛЕКУЛ

Резюме

Удосконалений комбінований теоретичний метод опису вібраційної структури для фотоелектронних спектрів молекул, який базується на методі функцій Гріна і теорії функціоналу густини , застосовано до кількісного опису фотоелектронного спектру двоатомних молекул. Густина станів, які описують коливальну структуру у фотоелектронних спектрах, визначається з використанням комбінованого Гріна підходу (метод функціоналу густини і функцій Гріна) та добре апроксимується з використанням тільки першого порядку констант зв'язку в одноквазічастинковому наближенні. Використання теорії функціоналу густини призводить до значного спрощення молекулярних розрахунків.

Ключові слова: фотоелектронний спектр молекул, метод функцій Гріна, теорія функціонала густини

UDC 621.396.67

A. O. Karpenko

Interdepartmental Scientific-Educational Physicotechnical Center of the Ministry of Education and Science and the National Academy of Sciences of Ukraine, I.I. Mechnikov National University. 2 Dvoryanskaya str. Odessa, 65082, Ukraine. e-mail: ndl_lepikh@onu.edu.ua

A METHOD FOR LOWERING THE LEVEL OF THE ELECTROMAGNETIC WAVES BACKGROUND RADIATION OF HORN RADIATOR

The problem about decrease in horn radiator electromagnetic waves return radiation level by a method of excitation of the slowed down surface waves on an exterior side of its aperture edge, being in an antiphase with return radiation electromagnetic waves has been solved.

For practical application of this method, a pyramidal H-sector horn radiator with curvilinear walls is taken. In the construction of this method, an impedance metal comb is used, which acts as a delay line for electromagnetic waves reflected from the aperture of the radiator.

Introduction

Horn radiators (HR) refer to an aperture class of the antenna working in a range of ultrahigh frequencies (UHF). Thanks to simplicity of a design and high technical characteristics HR have found wide application in modern radio-electronic communication systems, radar-locations, tele-radio broadcasting, and also in space flying vehicle.

One of HR advantages is the high radiation orientation which is characterised by the orientation diagramme (OD). HR have wide range of working frequencies, high efficiency and possibility to radiate electromagnetic waves of the big capacity (up to 100 MW) that make them irreplaceable in a radar-location and a space radio communication.

However, there are the various factors worsening HR characteristics. In particular:

1) sphericity of the phase front form in a plane of HR outlet aperture;

2) dispersion of the radiation basic harmonic field energy inside the HR on the set of mode of the higher harmonics;

3) occurrence of the electromagnetic field energy return reflexion in feeding wave guide;

4) occurrence of return radiation into the region of space which is behinde the HR.

The last is caused by a line of the phenomena in which number the most ponderable is the electromagnetic waves reradiation by the currents induced in the HR aperture outlet edge contour (aperture).

The researches [1-9] directed on improvement of HR characteristics have led to occurrence of HR new class with curvilinear walls in which influence of the listed phenomena is considerably reduced. However, the problem of the return radiation remains actual.

In our work the new method of the return radiation level arising on an edge of HR aperture outlet reduction which is applied to pyramidal HR with curvilinear walls is offered.

1. Problem statement

Let's consider cross-section of an aperture outlet of pyramidal HR, representing the electric contour of rectangular section K_1 radiating electromagnetic waves (fig. 1). Sources of an electromagnetic field are alternating currents i_1, i_2, i_3, i_4. Assume that each site of a contour radiates in space cylindrical waves with a length λ_0 and phase φ_0. Let's by condention, B - the area of direct radiation located in front of HR aperture . The plane of these areas section coincides with a plane of contour K_1. Let's place the geometrical centre of K_1 contour at the beginning of the co-

ordinate system. On an axis z in the region of semispace $A(-z, \pm x, \pm y)$ we will place contour K_2 identical to contour K_1 with the geometrical centre with coordinates $(0,0,-l)$.

Then the electromagnetic waves radiated by contour K_1 having passed distance l during t_{lag} will induce alternating currents i_1', i_2', i_3', i_4' in contour K_2. As the result the system of two radiating contours - active K_1 and passive K_2 will turn out, and the phase of radiation of a contour K_2 – φ_2 will lag behind phase φ_0 for time necessary for an electromagnetic wave for overcoming the distance l.

At axes z in a distant zone we will pick up the point $M_{z>>\lambda_0}$. The distance from zero of coordinate system to point $M_{z>>\lambda_0}$ should be 10 times more the wave length λ_0.

The electromagnetic waves radiated by contours K_1 and K_2 will reach point $M_{z>>\lambda_0}$ not simultaneously, and during $t_0 = \frac{R_1}{c}$ on radius-vector R_1 and $t_{lag} = \frac{l}{v} + \frac{R_2}{c}$, where v and c - electromagnetic waves speed of distribution between contours K_1 and K_2, and in free space accordingly. As R_1 and R_2 is more than distance between contours l it is possible to consider, that $R_1 = R_2 = R$.

It is necessary to define such time of delay t_{lag} at which in a point of supervision $M_{z>>\lambda_0}$ phases φ_0 and φ_2 will differ from each other on size π.

$$t_{lag} - t_0 = \pi \tag{1}$$

or

$$\frac{l}{v} - \frac{l}{c} = \frac{\lambda_0}{2c} \tag{2}$$

In this case the electric and magnetic field vectors radiated by contours K_1 and K_2 are in antiphase for any *x, y,-z* 10 times larger than λ_0 and the resultant capacity stream density in a distant zone of semispace A tends to zero. In semispace $B(z, \pm x, \pm y)$ in a distant zone phases φ_0 and φ_2 will coincide, as the wave passes between contours the distance equal 2*l* (there and back) for corresponding time $2t_{lag} = 2\pi$.

2. Decision technique

To fulfill conditions (1-2) it is necessary to reduce the electromagnetic energy distribution speed in the region $z(0, -l)$. For this purpose we will place between conductors of contours K_1 and K_2 the slowing down comb type structure made in the form of a flat metal comb (fig. 2).

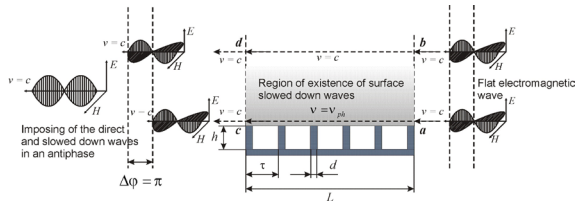


Fig. 2. A fragment of slowing down comb structure on the basis of an impedance metal comb. τ - the comb period, l – comb length, d – comb thickness, h – comb height , v - slowing down wave speed, v_{ph} - phase speed

The first comb (*a)* corresponds to contour K_1, the last comb (*c)* corresponds to contour K_2.

At interaction of a flat electromagnetic wave with an impedance metal comb over its surface the slowed down surface waves appear. Electrodynamics of the given process is studied enough [10-12]. Having solved the equation (2) concerning speed of the surface slowed down wave *v* we will receive:

$$v = c\frac{l}{\frac{\lambda_0}{2} + l} \tag{3}$$

Knowing the v size it is possible to find all geometrical parametres of slowing down structure, namely: τ - the comb period, l – the comb length , d –the comb thickness, h – the comb height at which the condition of formula (1) will be satisfied. Using received in [2, 10, 12] expressions for slowing down inductive type structure on the basis of an impedance metal comb we will write down the common decision of a problem uniting in geometrical and electrodynamic parametres.

$$\frac{c}{\sqrt{1+\left(\frac{\tau-d}{\tau}tg\frac{2\pi h_{\dot{y}}}{\lambda_0}\right)^2}}=\frac{lc}{\frac{\lambda_0}{2}+l};$$

$$\begin{cases} l=6\div 8\lambda_0; \\ \tau<0{,}5\lambda_0; \\ d<<\tau; \\ 0<h_{eff}<\dfrac{\lambda_{max}}{4}. \end{cases} \quad (4)$$

where c - speed of electromagnetic waves distribution in vacuum;

λ_0 - length of a wave corresponding to the middle of the operating band;

λ_{max} - maximum length of a wave of the operating band;

λ_{min} - minimum length of a wave of the operating band;

τ - comb period;

d - comb thickness;

l – comb length;

h_{eff} – combs effective height counted under the formula:

$$h_{eff}=h-0.14\left(d+\tau\right),$$

where h – the constructive (in fact) edge height.

3. Results and discussion

For practical application described above method it is taken pyramidal N-sectorial HR with curvilinear walls, in which design the impedance metal comb is included (fig. 3).

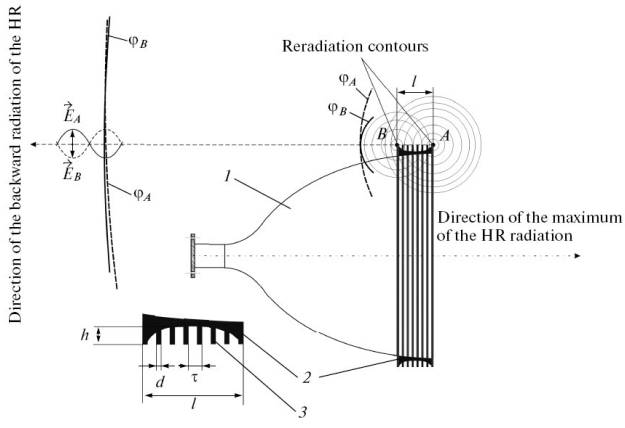


Fig. 3. H-sectorial HR with curvilinear walls of combined form with the return radiation lowered level. 1-H-sectorial HR with curvilinear walls of combined forms, 2- comb type slowing down structure in the form of a flat metal impedance comb in section, 3 - metal comb edge, l - metal comb length, τ - the comb-period, d – comb thickness, h – comb height

The prototype sample of offered HR with following parametres is made and tested:

- the minimum wavelength of the operating band $\lambda_{\min}=24$ mm;
- the maximum wavelength of operating band $\lambda_{\max}=36$ mm;
- the length of a horizontal rib of HR outlet aperture A_p = 100 mm;
- the rib constructive height h=3 mm;
- the edge thickness d = 0,5 mm;
- the comb period τ = 5 mm;
-the comb length l = 210 mm;
- Metal comb flutes depth changes on exponential law.

In polar system of coordinates are constructed normalized directional diagrames (DD) of HR prototype sample (solid line) and similar HR, but without impedance comb (dotted line) (fig. 4).

4. Conclusions

The analysis of received DD allows to conclude.

1. Level of back lobe DD of HR prototype sample with an impedance comb is considerably less, than at HR without an impedance comb;

2. At observation angle of $\theta = 90^0$ concerning the radiation maximum in developed HR intensity of an electromagnetic field decreases, and at HR without an impedance comb, on the contrary, in the given point growth of intensity of an electromagnetic field is observed. Theoretical calculations and experimental researches of HR sample confirm efficiency of the offered decision.

References

1. Karpenko A.A. Yssledovanye rupornykh yzluchateley po dyapazonnыm svoystvam // Odesa: Haykovi pratsi UDAZ im. O. S. Popova, 2000., №1., S. 76-77.
2. Karpenko A.A., Lepikh Ya.I. Kompensatsyya fazovoy oshybky v yzluchatelyakh SVCh-voln s pomoshch'yu ympedansnoy struktury // Tekhnolohyya y konstruyrovanye v elektronnoy apparature. 2007., Odesa, №2 (68), S. 38-41.
3. Karpenko A.A., Lepikh Ya.I. Yzluchatel' elektromahnytnykh voln s kombynyrovannoy formoy obrazuyushchykh // Radyotekhnyka i elektronyka. Tom 53., № 7., 2008., Moskva., S. 818-824.
4. Karpenko A.A., Lepikh Ya.I. Metod rascheta rupornoho pyramydal'noho yzluchatelya voln SVCh s kryvolyneynoy obrazuyushchey // Radyoelektronyka. Yzvestyya visshykh uchebnykh zavedenyy KNTU. Tom 51., № 5-6., 2008., Kyev., S. 22-33.
5. Karpenko A.O., Lepikh Ya.I. Vyprominyuvach elektromahnitnykh khvyl' NVCh diapazonu z kerovanym fazovym frontom. Patent na korysnu model' UA № 53694 (51)MPK (2009) H01Q 13/00
6. Karpenko A.O., Lepikh Ya.I. Vyprominyuvach elektromahnitnykh khvyl'. Patent UA №97300 (51)MPK (2012) H01Q 13/02 (2006.01)
7. Karpenko A.O., Lepikh Ya.I. Rupornyy piramidal'nyy vyprominyuvach elektromahnitnykh khvyl' NVCh diapazonu. Patent UA №75105 (51) MPK (2012.01) H01Q 13/00
8. Shumlyanskyy I.I. // Rupornye yzluchately so stupenchatыmy y kryvolyneynymy obrazuyushchymy.– K.: Vyshcha shk. Holovnoe yzd-vo, 1986. – 147s.
9. I.I. Shumljansky. Horn radiators of complex configuration. Copyright 1993 by World Scientific Publishing Singapore, New Jersey, London, Hon Kong. Co. Pte. Ltd.
10. Benenson L.S., Kyurkchan A.H. Metod razvyazky antenn pry pomoshchy peryodycheskykh struktur // Radyotekhnyka.– 1995.– № 12.– s. 62–69.
11. Lobkova L.M. Proektyrovanye antenn y ustroystv SVCh: Ucheb. posobye dlya vuzov / L.M. Lobkova. – Sevastopol': Yzd-vo SevNTU, 2002. – 178 s.
12. Habryl'yan D.D., Zvezdyna M.Yu., Kostenko P.Y. Umen'shenye bokovoho y zadneho yzluchenyya antenny na osnove yspol'zovanyya ympedansnykh struktur. // Radyoelektronyka.–2003.– № 2.– s.38 - 43.

This article has been received in April 2017

UDC 621.396.67

A. O. Karpenko

A METHOD FOR LOWERING THE LEVEL OF THE ELECTROMAGNETIC WAVES BACKGROUND RADIATION OF HORN RADIATOR

Summary

The problem about decrease in horn radiator electromagnetic waves return radiation level by a method of excitation of the slowed down surface waves on an exterior side of its aperture edge, being in an antiphase with return radiation electromagnetic waves has been solved.

For practical application of this method, a pyramidal H-sector horn radiator with curvilinear walls is taken. In the construction of this method, an impedance metal comb is used, which acts as a delay line for electromagnetic waves reflected from the aperture of the radiator.

Key words: Horn radiator, horn antenna, surface electromagnetic waves, impedance retardation structure, radiation pattern

УДК 621.396.67

А. А. Карпенко

МЕТОД СНИЖЕНИЯ УРОВНЯ ОБРАТНОГО ИЗЛУЧЕНИЯ ЭЛЕКТРОМАГНИТНЫХ ВОЛН РУПОРНОГО ИЗЛУЧАТЕЛЯ

Аннотация

Решена задача о снижении уровня обратного излучения электромагнитных волн рупорного излучателя методом возбуждения замедленных поверхностных волн на внешней стороне кромки его раскрыва, находящихся в противофазе с электромагнитными волнами обратного излучения.

Для практического применения данного метода взят пирамидальный Н-секториальный рупорный излучатель с криволинейными стенками, в конструкцию которого включена импедансная металлическая гребёнка, выполняющая роль линии задержки для отраженных от апертуры излучателя электромагнитных волн.

Ключевые слова: Рупорный излучатель, рупорная антенна, поверхностные электромагнитные волны, импедансная замедляющая структура, диаграмма направленности.

УДК 621.396.67

А. О. Карпенко

МЕТОД ЗНИЖЕННЯ РІВНЯ ЗВОРОТНОГО ВИПРОМІНЮВАННЯ РАДІОХВИЛЬ РУПОРНОГО ВИПРОМІНЮВАЧА

Аннотація

Розв’язана задача про зниження рівня зворотного випромінювання електромагнітних хвиль рупорного випромінювача шляхом збудження уповільнених поверхневих хвиль на зовнішній стороні кромки його розкриву, що знаходяться в протифазі з електромагнітними хвилями зворотного випромінювання.

Для практичного застосування даного методу взято пірамідальний Н-секторіальний рупорний випромінювач з криволінійними стінками, в конструкцію якого включена імпедансна металева гребінка, що виконує роль лінії затримки для відбитих від апертури випромінювача електромагнітних хвиль.

Ключові слова: Рупорний випромінювач, рупорна антена, поверхневі електромагнітні хвилі, імпедансна уповільнююча структура, діаграма направленості.

UDC 539.187

V. V. Buyadzhi, Yu. G. Chernyakova, O. A. Antoshkina, T. B. Tkach

Odessa State Environmental University, 15, Lvovskaya str., Odessa-16, 65016, Ukraine
E-mail: buyadzhivv@gmail.com

SPECTROSCOPY OF MULTICHARGED IONS IN PLASMAS: OSCILLATOR STRENGTHS OF Be-LIKE ION Fe

The generalized relativistic energy approach with using the Debye shielding model is used for studying spectral parameters of ions in plasma and determination of the oscillator strengths for the Be-like ions. An electronic Hamiltonian for N-electron ion in a plasma is added by the Yukawa-type electron-electron and nuclear interaction potential. Oscillator strengths gf for $2s^2$-$[2s_{1/2}2p_{3/2}]_1$ transition in Be-like Fe are computed for different values of the electron density and temperature (n_e=10^{22}-10^{24}cm^{-3}, T=0.5-2 keV) of plasmas are presented and compared with available alternative spectroscopic data.

1. Introduction

Spectroscopy of multicharged ions in a plasmas is one of the most fast developing branches of modern atomic spectroscopy. Let us remind that a great interest to studying radiation and collision processes parameters in a plasmas is connected with importance of these data for correct description of parameters characteristics for plasma in thermonuclear (tokamak) reactors, searching new mediums for X-ray range lasers [1-20]. In many papers the calculations of various atomic systems embedded in Debye plasmas have been performed ([13-16]). Different theoretical methods were employed along with the Debye screening to study plasma medium. Earlier we have developed a new version of a relativistic energy approach combined with the many-body perturbation theory (RMBPT) for multi-quasiparticle (QP) systems for studying spectra of plasma of the multicharged ions and electron-ion collisional parameters. The method is based on the Debye shielding model and energy approach [16-22]. A new element of this paper is in using the effective optimized Dirac-Kohn-Sham method in general relativistic energy approach to collision processes in the Debye plasmas. Here Oscillator strengths gf for $2s^2$-$[2s_{1/2}2p_{3/2}]_1$ transition in Be-like Fe are computed for different values of the electron density and temperature (n_e=10^{22}-10^{24}cm^{-3}, T=0.5-2 keV) of plasmas are presented and compared with available alternative spectroscopic data.

2. Generalized energy approach in scattering theory. Debye shielding model

Let us firstly consider the Debye shielding model accordinf to Refs. [16,18]. It is known (see [10-14,19] and refs. therein) in the classical theory of plasmas developed by Debye-Hückel, the interaction potential between two charged particles is modelled by the Yukawa-type potential, which contains the shielding parameter m [1]. The parameter m is connected with the plasma parameters such as the temperature T and the charge density n as follows: $\mu \sim \sqrt{e^2 n / k_B T}$. Here, as usually, e is the electron charge and $\kappa_Б$ is the Boltzman constant. The density n is given as a sum of the electron density N_e and ion density N_k of the k-th ion species having the nuclear charge q_k : $n = N_e + \sum_k q_k^2 N_k$. Under typical laser plasma conditions of T~1keV and n~10^{22} cm^{-3} the parameter m is of the order of 0.1 in atomic units [13,14]. By introducing the Yukawa-type e-N and e-e interaction potentials, an electronic Hamiltonian for N-electron ion in a plasma is in atomic units as follows [19]:

$$H = \sum_i [\alpha cp - \beta mc^2 - Z\exp(-\mu r_i)/r_i] + \\ + \sum_{i>j} \frac{(1-\alpha_i\alpha_j)}{r_{ij}} \exp(-\mu r_{ij}) \quad (1)$$

The generalized relativistic energy approach combined with the RMBPT has been in details described in Refs. [19-22]. It generalizes earlier developed energy approach [5-8]. The key idea is in calculating the energy shifts D*E* of degenerate states that is connected with the secular matrix *M* diagonalization [4-6]. To construct *M*, one should use the Gell-Mann and Low adiabatic formula for D*E*. The secular matrix elements are already complex in the PT second order. The whole calculation is reduced to calculation and diagonalization of the complex matrix *M* .and definition of matrix of the coefficients with eigen state vectors $B^K_{ie,iv}$ [5-8]. To calculate all necessary matrix elements one must use the basis's of the 1QP relativistic functions. Within an energy approach the total energy shift of the state is usually presented as [3-7]:

$$\Delta E = \mathrm{Re}\Delta E + i\,\Gamma/2 \quad (2)$$

where *G* is interpreted as the level width and decay possibility *P* = *G*. The imaginary part of electron energy of the system, which is defined in the lowest PT order as [3]:

$$\mathrm{Im}\Delta E(B) = -\frac{e^2}{4\pi} \sum_{\substack{\alpha>n>f \\ [\alpha<n\le f]}} V^{|\omega_{\alpha n}|}_{\alpha n \alpha n}, \quad (3)$$

where $\sum_{\alpha>n>f}$ for electron and $\sum_{\alpha<n\le f}$ for vacancy. The separated terms of the sum in (3) represent the contributions of different channels and a probability is:

$$\Gamma_{\alpha_n} = \frac{1}{4\pi} \cdot V^{|\omega_{\alpha_n}|}_{\alpha_n \alpha_n} \quad (4)$$

Which is linked with an oscillator strength by the standard way. It is known that their adequate description requires using the optimized basis's of wave functions. In [6] it has been proposed "ab initio" optimization principle for construction of cited basis's. It uses a minimization of the gauge dependent multielectron contribution of the lowest QED PT corrections to the radiation widths of atomic levels. This contribution describes collective effects and it is dependent upon the electromagnetic potentials gauge (the gauge non-invariant contribution dE_{ninv}). The minimization of ImdE_{ninv} leads to integral differential equation, that is numerically solved. In result one can get the optimal one-electron basis of the PT [21-23]. It is worth to note that this approach was used under solvin of multiple problems of modern atomic , nuclear and molecular physics (see [23-67]). To generate the wave functions basis we use the optimized Dirac-Kohn-Sham potential with one parameter [8], which calibrated within the special ab initio procedure within the relativistic energy approach [6]. The modified PC numerical code 'Superatom" is used in all calculations. Other details can be found in Refs. [5-9, 16-22].

3. Results and conclusion

Firstly, we present our results on energy shifts and oscillator strengths for transitions $2s^2$-$2s_{1/2}2p_{1/2,3/2}$ in spectra of the Be-like Fe. The corresponding plasma parameters are as follows: $n_e=10^{22}$-10^{24}cm^{-3}, T=0.5-2 keV (i.e. m~0.01-0.3). We studied a behavior of the energy shifts DE (cm^{-1}) for $2s^2$-$[2s_{1/2}2p_{1/2,3/3}]_1$ transitions and oscillator strengths changes for different plasma parameters (the electron density and temperature). In Table 1 there are listed the oscillator strengths gf for $2s^2$-$[2s_{1/2}2p_{3/2}]_1$ transition in Be-like Fe for different values of the n_e (см$^{-3}$) and T (in eV).

Table 1

Oscillator strengths for $2s^2$-$[2s_{1/2}\,2p_{3/2}]_1$ transition in Be-like Fe for different n_e (см$^{-3}$) and T (eV) (gf_0 –gf value for free ion)

n_e		10^{22}	10^{23}	10^{24}
kT	[13]	[13]	[13]	[13]
500	0.1537	0.1537	0.1538	0.1547
1000		0.1537	0.1538	0.1545
2000		0.1537	0.1538	0.1543

Продовження таблиці 1

2000		0.1555	0.1556	0.1562
I-S		0.1537	0.1537	0.1540
		0.1555	0.1555	0.1559
n_e		10^{22}	10^{23}	10^{24}
kT	Our	Our	Our	Our
500	0.1541	0.1541	0.1543	0.1553
1000		0.1541	0.1543	0.1553
2000		0.1540	0.1542	0.1552
2000		0.1541	0.1542	0.1552

There are also listed the available data by Li etal and Saha-Frische: the multiconfiguration Dirac-Fock (DF) calculation results, and ionic sphere (I-S) model simulation data [13, 16] (see refs. therein). The analysis shows that the presented data are in physically reasonable agreement, however, some difference can be explained by using different relativistic orbital basises and different models for accounting of the plasma screening effect. It is important to note that our computing oscillator strengths within an energy approach with different forms of transition operator (this is corresponding to using the photon propagators in the form of Coulomb, Feynman and Babushkin) gives very close results.

References

1. Oks E., Stark Broadening of Hydrogen and Hydrogenlike Spectral Lines in Plasmas: The Physical Insight (Oxford: Alpha Science International).-2006.
2. Griem H R , Spectral Line Broadening by Plasmas(N.-Y.: Academic Press).-1974.
3. Oks E., Relation between theories, experi-ments, and simulations of spectral line shapes //Int.J.Spectr.-2010.-Vol.10.-P. 852581.
4. Ivanova E.P., Grant I., Oscillator strength anomalies in Ne isoelectronic sequence with applications to X-ray laser modeling// J. Phys. B:At.Mol.Phys.-1998-Vol.31.-P.2871-2883
5. Ivanov L.N., Ivanova E.P., Knight L., Energy Approach to consistent QED theory for calculation of electron-collision strengths/ //Phys.Rev.A.-1993.-Vol.48.-P.4365-4374.
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(1).-P.33-36.
7. Glushkov A.V.,Ivanov L.N., DC Strong-Field Stark-Effect: consistent quantum-mechanical approach//J.Phys.B:At. Mol.Opt.Phys.-1993.-Vol.26.-P.L379-386.
8. Glushkov A.V., Relativistic Quantum Theory. Quantum, mechanics of Atomic Systems.-Odessa: Astroprint, 2008.-700P.
9. Ivanov L.N.,Ivanova E.P., Extrapolation of atomic ion energies by model potential method: Na-like spectra// Atom. Data Nucl Data Tab.-1999.-Vol.24.-P.95-121.
10. Khakoo M.A., Wrkich J., Larsen M. et al, Differential cross-sections and cross-sections ratios for the electron-impact excitation of the neon $2p^5 3s$ configuration//Phys.Rev.A.-2002.-Vol.65.-P.062711.
11. Khakoo M.A., Vandeventer P., Childers J.G. etal, Electron-impact excitation of argon $3p^5 4s$ configuration: Differential cross-sections and cross-sections ratios// J. Phys. B: At. Mol. Phys.-2004.-Vol.37.-P.247-281.
12. Griffin D., Balance C., Mitnik D., Berengut J., Dirac R-matrix calculations of electron-impact excitation of Ne-like Kr//J.Phys.B: At. Mol. Opt. Phys.-2008.-Vol.41.-P.215201.
13. Yongqiang Li, JianhuaWu, Yong Hou, Jianmin Yuan, Influence of hot and dense plasmas on energy levels& oscillator strengths of Be-like ions for Z = 26–36// J. Phys. B: At. Mol. Opt. Phys.-2008.-Vol.41.-P.145002.
14. Okutsu H., SakoI., Yamanouchi K., Di-

ercksen G., Electronic structure of atoms in laser plasmas: Debae shielding approach// J.Phys. B: At. Mol.Phys.-2005-Vol.38.-P.917-927.
15. Smith A., Bannister M., Chung Y., Djuric N., Dunn G., Wallbank B., Woitke O., Near-threshold electron-impact excitation of multiply-charged Be-like ions//Phys.Scr.-1999.-Vol.T80-P.283-287.
16. Buyadzhi V.V., Chernyakova Yu.G., Smirnov A.V., Tkach T.B., Electron-collisional spectroscopy of atoms and ions in plasma: Be-like ions// Photoelectronics.-2016.-Vol.25.-P.97-101.
17. Malinovskaya S.V., Glushkov A.V., Khetselius O.Yu., Lopatkin Yu., Loboda A.V., Svinarenko 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,N2.-P.288-296.
18. Malinovskaya S.V., Glushkov A.V., Khetselius O.Yu., Svinarenko A.A., Mischenko E.V., Florko T.A., Optimized perturbation theory scheme for calculating the interatomic potentials and hyperfine lines shift for heavy atoms in the buffer inert gas//Int. J. Quant. Chem.-2009.-Vol.109.-P.3325-3329.
19. 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.
20. 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.
21. 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.
22. 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
23. 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.
24. Glushkov A.V., Energy approach to resonance states of compound super-heavy nucleus and EPPP in heavy nucleus collisions// Low Energy Antiproton Phys. AIP Conference Proceedings.-2005.-Vol.796.-P.206-210.
25. 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.
26. 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.
27. 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.
28. 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. J. Quant. Chem.-2004.-Vol.99.-P.889-893.
29. 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.
30. 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
31. Glushkov A.V., Ambrosov S.V., Loboda A.V., Gurnitskaya E.P., Khetselius O.Yu., QED calculation of heavy multicharged ions with account for the correlation, radiative and nuclear effects// Recent Advances in Theor. Phys. and Chem. Systems.-2006.-Vol.15.-P.285-300.
32. 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.
33. 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 shileding approximation// Sensor Electr. and Microsyst. Techn.-2007.-N2.-P.9-13
34. 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.
35. 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.
36. 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.
37. 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.
38. Glushkov A.V., Relativistic and correlation effects in spectra of atomic systems.-Odessa: Astroprint.-2006.-400P.
39. Glushkov A.V., Atom in electromagnetic field.-Kiev: KNT, 2005.-450P.
40. Khetselius O.Yu., Hyperfine structure of atomic spectra.-Odessa: Astroprint, 2008.-210P.
41. Khetselius O.Yu., Hyperfine structure of radium// Photoelectronics.-2005.-N14.-P.83-85.
42. Khetselius O., Spectroscopy of cooperative electron-gamma-nuclear processes in heavy atoms: NEET effect// J. Phys.: Conf. Ser.-2012.- Vol.397.-P.012012
43. 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.

44. 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.
45. 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.
46. Glushkov A., Malinovskaya S., Gurnitskaya E., Khetselius O.Yu.,Dubrovskaya Yu., 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.
47. Glushkov A.V., Khetselius O.Y., Brusentseva S.V., Zaichko P.A., Ternovsky V.B., Studying interaction dynamics of chaotic systems within a nonlinear prediction method: application to neurophysiology// Advances in Neural Networks, Fuzzy Systems and Artificial Intelligence, Ser: Recent Adv. in Computer Engineering, Ed. J.Balicki.-2014.-Vol.21.-P.69-75.
48. Khetselius O.Yu., Quantum Geometry: New approach to quantization of the quasistationary states of Dirac equation for super heavy ion and calculating hyper fine structure parameters// Proc. Int. Geometry Center.-2012.-Vol.5,№ 3-4.-P.39-45.
49. 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.
50. 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.
51. 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.
52. 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. Proc.-2008.-Vol.1058.-P.231-233.
53. Khetselius O.Yu., Hyperfine structure of energy levels for isotopes 73Ge, 75As, 201Hg// Photoelectronics.-2007.-N16.-P.129-132.
54. 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.
55. 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.
56. 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.
57. 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.
58. Glushkov A.V., Khetselius O.Yu., Kuzakon V., Prepelitsa G.P., Solyanikova E.P., Svinarenko A., Modeling of interaction of the non-linear vibrational systems on the basis of temporal series analyses (application to semiconductor quantum generators)// Dynamical Systems-Theory and Applications.-2011.-BIF110.
59. Svinarenko A.A., Nikola L. V., Prepelitsa G., Tkach T.B, Mischenko E.V.,

Auger (autoionization) decay of excited states in spectra of multicharged ions: Relativistic theory//AIP Conf. Proc.-2010.-Vol.1290, N1 P.94-98.
60. 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.-525-541.
61. 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.
62. Glushkov A.V., Khetselius O., Svinarenko 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.
63. 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.
64. 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.
65. Glushkov A.V., Khetselius O.Yu., Prepelitsa G., 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 International Geometry Center».-2013.-Vol.6, N1.-P.43-48.
66. 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.
67. 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.

This article has been received in May 2017

UDC 539.187

V. V. Buyadzhi, Yu. G. Chernyakova, O. A. Antoshkina, T. B. Tkach

SPECTROSCOPY OF MULTICHARGED IONS IN PLASMAS: OSCILLATOR STRENGTHS OF Be-LIKE ION Fe

Summary

The generalized relativistic energy approach with using the Debye shielding model is used for studying spectral parameters of ions in plasma and determination of the oscillator strengths for the Be-like ions. An electronic Hamiltonian for N-electron ion in a plasma is added by the Yukawa-type electron-electron and nuclear interaction potential. Oscillator strengths gf for $2s^2$-$[2s_{1/2}2p_{3/2}]_1$ transition in Be-like Fe are computed for different values of the electron density and temperature ($n_e=10^{22}$-$10^{24}cm^{-3}$, T=0.5-2 keV) is presented and compared with available alternative spectroscopic data.

Key words: spectroscopy of ions in plasmas, relativistic energy approach, oscillator strengths

УДК 539.187

В. В. Буяджи, Ю. Г. Чернякова, О. А. Антошкина, Т. Б. Ткач

СПЕКТРОСКОПИЯ МНОГОЗАРЯДНЫХ ИОНОВ В ПЛАЗМЕ: СИЛЫ ОСЦИЛЛЯТОРОВ ДЛЯ Be-ПОДОБНОГО ИОНА Fe

Резюме

На основе обобщенного релятивистского энергетического подхода с использованием модели экранирования Дебая выполнено изучение спектра плазмы ионов и определение сил осцилляторов для Be-подобных ионов. Электронный гамильтониан для N-электронного иона в плазме дополнен потенциалом электрон-электронного и ядерного взаимодействия типа Юкавы. Силы осцилляторов $2s^2$-$[2s_{1/2}2p_{3/2}]_1$ перехода в Be-подобном Fe определены для различных значений электронной плотности и температуры ($n_e=10^{22}$-$10^{24}cm^{-3}$, T=0.5-2 keV) плазмы и сравниваются с имеющимися альтернативными спектроскопическими данными. .

Ключевые слова: спектроскопия ионов в плазме, энергетический подход, силы осцилляторов

УДК 539.187

В. В. Буяджи, Ю. Г. Чернякова, О. О. Антошкіна, Т. Б. Ткач

СПЕКТРОСКОПІЯ БАГАТОЗАРЯДНИХ ІОНІВ В ПЛАЗМІ: СИЛИ ОСЦИЛЯТОРІВ ДЛЯ Be-ПОДІБНОГО ІОНА Fe

Резюме

На основі узагальненого релятивістського енергетичного підходу з використанням моделі екранювання Дебая виконано вивчення спектру плазми іонів і визначення сил осциляторів для Be-подібних іонів. Електронний гамильтоніан для N-електронного іона в плазмі доповнений потенціалом електрон-електронної та ядерної взаємодії типу Юкави. Сили осциляторів $2s^2$-$[2s_{1/2}2p_{3/2}]_1$ переходу в Be-подібному Fe визначені для різних значень електронної густини і температури ($n_e=10^{22}$-$10^{24}cm^{-3}$, T=0.5-2 keV) плазми та порівнюються з наявними альтернативними спектроскопічними даними.

Ключові слова: спектроскопія іонів в плазмі, енергетичний підхід, сили осциляторів

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 $\mathrm{Re}\,\Delta E$ calculation procedure has been generalized for the case of nearly degenerate states, whose levels form a more or less compact group. One of these variants has been previously [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 $\mathrm{Re}\,M^{(2)}$ 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 $\mathrm{Re}R_\lambda(1243)$ 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 $f/r^{|æ|-1}$, $g/r^{|æ|-1}$, $Z_\lambda^{(1)}$, $Z_\lambda^{(2)}$. 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 $4f^{13}$ $[^2F_{7/2}]6s^2np[5/2]_2$ and $4f^{13}$ $[^2F_{7/2}]$ $6s^2$ 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 $4f^{13}$ $[^2F_{7/2}]$ $6s^2\,nf\,[5/2]_2$ 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 $4f^{13}$ $[^2F_{7/2}]6s^2np[5/2]_2$ 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 $4f^{13}$ $[^2F_{7/2}]$ $6s^2$ 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.Brändas, 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 multicharged 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 cooperative 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 hyper fine 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.

UDC 539.182

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

ТЕОРЕТИЧЕСКОЕ ИЗУЧЕНИЕ СПЕКТРА АТОМА ИТЕРБИЯ НА ОСНОВЕ РЕЛЯТИВИСТСКОЙ МНОГОЧАСТИЧНОЙ ТЕОРИИ ВОЗМУЩЕНИЙ: РИДБЕРГОВЫ РЕЗОНАНСЫ

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

ТЕОРЕТИЧНЕ ВИВЧЕННЯ СПЕКТРА АТОМА ІТЕРБІЮ НА ОСНОВІ РЕЛЯТИВІСТСЬКОЇ БАГАТОЧАСТИНКОВОЇ ТЕОРІЇ ЗБУРЕНЬ: РІДБЕРГОВІ РЕЗОНАНСИ

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

UDC 539.182

A. V. Smirnov, O. Yu. Khetselius, V. V. Buyadzhi, A. S. Belodonov

Odessa State Environmental University, 15, Lvovskaya str., Odessa, Ukraine
E-mail: smirnovandvla@gmail.com

ADVANCED RELATIVISTIC APPROACH IN SPECTROSCOPY OF COMPLEX AUTOIONIZATION RESONANCES IN ATOMIC SPECTRA

We applied a generalized energy approach (Gell-Mann and Low S-matrix formalism) combined with the relativistic multi-quasiparticle (QP) perturbation theory (PT) with the Dirac-Kohn-Sham zeroth approximation and accounting for the exchange-correlation, relativistic corrections to studying autoionization resonances in the helium spectrum, in particular, we predicted the energies and widths of the number of the Rydberg resonances. There are presented the results of comparison of our theory data for the autoionization resonance 3s3p 1P0 with the available experimental data and those results of other theories, including, method of complex rotation by Ho, algebraic approach by Wakid-Callaway, diagonalization method by Senashenko-Wague etc.

1. Introduction

The knowledge of autoionization states properties of atomic systems is of a great importance note for many applications in atomic and molecular physics, plasma chemistry and physics, laser physics and quantum electronics etc. [1-52]. In this paper, which goes on our studying autoionization phenomena in different atomic systems, we present an advanced new relativistic approach [11-15] to relativistic calculating autoionization resonances (AR) characteristics of the helium atom. The new elements of the approach include the combined the generalized energy approach and the gauge-invariant relativistic many-body perturbation theory (PT) with the Dirac-Kohn-Sham (DKS) "0" approximation (optimized 1QP representation) and an accurate accounting for relativistic, correlation and others effects. The generalized gauge-invariant version of the energy approach has been further developed in Refs. [12,13].

2. Relativistic perturbation theory approach in spectroscopy of autoionization states

In refs. [11-15, 17-20] the fundamentals of the relativistic many-body PT formalism have been in details presented, so further we are limited only by the novel elements. Let us remind that the majority of complex atomic systems possess a dense energy spectrum of interacting states. In refs. [11-15, 17-20] it is realized a field procedure for calculating the energy shifts ΔE of degenerate states, which is connected with the secular matrix *M* diagonalization [8-12]. The whole calculation of the energies and decay probabilities of a non-degenerate excited state is reduced to the calculation and diagonalization of the *M*. The complex secular matrix *M* is represented in the form [9,10]:

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

where $M^{(0)}$ is the contribution of the vacuum diagrams of all order of PT, and $M^{(1)}$, $M^{(2)}$, $M^{(3)}$ those of the one-, two- and three-QP diagrams respectively. The diagonal matrix $M^{(1)}$ can be presented as a sum of the independent 1QP contributions. The optimized 1-QP representation is the best one to determine the zeroth approximation. In the second order, there is important kind of diagrams: the ladder ones. These contributions have been summarized by a modification of the central potential, which must now include the screening (anti-screening) effect of each particle by two others. The additional potential modifies the 1QP orbitals and energies.

A width of a state associated with the decay of the AR is determined by square of the matrix element of the interparticle interaction $\Gamma \infty |V(\beta_1\beta_2, \beta_3 k)|^2$. The total width is given by the expression:

$$\Gamma(n_1^0 j_1^0, n_2^0 j_2^0; J) = \frac{2\pi}{K_0} \sum_{\beta_1\beta_2} \sum_{\beta_1'\beta_2'} C^J(\beta_1\beta_2) \times$$

$$\times C^J(\beta_1'\beta_2') \sum_{\beta\,\beta_K} V_{\beta_1\beta_2;\beta\,\beta_K} V_{\beta_K\beta\,;\beta_1'\beta_2'} \qquad (2)$$

where the coefficients C are in details described, for example, in Refs. [1-5]. The matrix element of the relativistic inter-particle interaction

$$V(r_i r_j) = exp(iù_j r_j) \cdot (1 - á_i á) / r_j \qquad (3)$$

(here α_I –the Dirac matrices) in (3) is determined as follows:

$$V_{\beta_1\beta_2;\beta_4\beta_3} = \sqrt{(2j_1+1)(2j_2+1)(2j_3+1)(2j_4+1)} \times$$

$$\times (-1)^{j1+j2+j3+j4+m1+m2} \times \qquad (4)$$

$$\text{x} \sum_{a\mu} (-1)^{\mu} \begin{pmatrix} j_1 & j_3 & a \\ m_1 & -m_3 & \mu \end{pmatrix} \begin{pmatrix} j_2 & j_4 & a \\ m_2 & -m_4 & \mu \end{pmatrix} \times$$

$$\times Q_a(n_1 l_1 j_1 n_2 l_2 j_2; n_4 l_4 j_4 n_3 l_3 j_3),$$

$$Q_a = Q_a^{\text{Qul}} + Q_a^{\text{B}} \,. \qquad (5)$$

Here Q_a^{Qul} and Q_a^{B} is corresponding to the Coulomb and Breit parts of the interparticle interaction (5). The calculating of all matrix elements, wave functions, Bessel functions etc is reduced to solving the system of differential equations. The formulas for the autoionization (Auger) decay probability include the radial integrals $R_\alpha(\alpha k \gamma \beta)$, where one of the functions describes electron in the continuum state. When calculating this integral, the correct normalization of the wave functions is very important, namely, they should have the following asymptotic at $r \to 0$:

$$\left.\begin{matrix} f \\ g \end{matrix}\right\} \to (\lambda\omega)^{-1/2} \begin{cases} \left[\omega + (\alpha Z)^{-2}\right]^{-1/2} sin(kr + \delta), \\ \left[\omega - (\alpha Z)^{-2}\right]^{-1/2} cos(kr + \delta). \end{cases} \qquad (6)$$

The important aspect of the whole procedure is an accurate accounting for the exchange-correlation effects. We have used the generalized relativistic Kohn-Sham density functional [33-35] in the zeroth approximation of relativistic PT; naturally, the perturbation operator contents the operator (3) minus the cited Kohn-Sham density functional. Further the wave functions are corrected by accounting of the first order PT contribution. Besides, we realize the procedure of optimization of relativistic orbitals base. The main idea is based on using ab initio optimization procedure, which is reduced to minimization of the gauge dependent multielectron contribution $Im\delta E_{ninv}$ of the lowest QED PT corrections to the radiation widths of atomic levels. According to [35-37], "in the fourth order of QED PT (the second order of the atomic PT) there appear the diagrams, whose contribution to the $Im\delta E_{ninv}$ accounts for correlation effects and this contribution is determined by the electromagnetic potential gauge (the gauge dependent contribution)". The accurate procedure for minimization of the functional $Im\delta E_{ninv}$ leads to the Dirac-Kohn-Sham-like equations for the electron density that are numerically solved by the Runge-Cutta standard method It is very important to known that the regular realization of the total scheme allow to get an optimal set of the 1QP functions and more correct results in comparison with so called simplified one, which has been used in Refs. [34-34] and reduced to the functional minimization using the variation of the correlation potential parameter *b*. Other details can be found in refs.[10-13,16-20,41-74] as well as description of the "Superatom" and Cowan PC codes, used in all computing.

3. Results and conclusion

In the Table 1 we present the comparison of our advanced data for the AR 3s3p $^1P_0$ with those of other theories, including, method of complex rotation by Ho, algebraic approach by Wakid-Callaway, diagonalization method by Senashen-

ko-Wague, relativistic Hartree-Fock (RHF) method by Nicolaides-Komninos, R-matrix method by Hayes-Scott, method of the adiabatic potential curves by Koyoma-Takafuji-Matsuzawa and Sadeghpour, L^2 technique with the Sturm decomposition by Broad- Gershacher and Moccia-Spizzo, the Feshbach method by Wu-Xi) and data measurements in laboratories: NIST (NBS; 2SO-MeV electron synchrotron storage ring (SURF-II)), Wisconsin Laboratory (Wisconsin Tantalus storage ring), Stanford Synchrotron Radiation Laboratory (SSRL), Berlin electron storage ring (BESSY), Daresbury Synchrotron Radiation Source (DSRS) [1,3,5,22-24].

Table 1a

Theoretical data for energy of the AR 3s3p $^1P_0$ (our data with those of other theories)

Method/Data	Er (eB)	Γ/2 (eB)
Our	69.9113	0.1912
ACC	69.8892	0.1891
Diagon. method	69.9096	0.1491
RHF	69.8703	-
APC1	69.8103	-
L^2 tech.	69.8737	0.1915
Feshbach th.	69.8991	0.1143
K-matrix L^2	69.8788	0.1839
PT- Svin	69.9055	0.1854
CR method	69.8722	0.1911
MC HF	69.8703	-
R-matrix	69.8797	0.1796
E:Wisconsin	69.917±0.012	0.178±0.012
E: SSRL-1987	69.917±0.012	0.178±0.012
E: BESSY	69.914±0.015	0.200±0.020
E: DSRS	69.880±0.022	0.180±0.015

Note: ACC- Algebraic close coupling; APC - Adiabatic potential curves; CR method-method of complex rotation; DM method – Diagonalization method

On the one hand, there is sufficiently good accuracy of our theory, the secondly (bearing in mind that most of the listed methods are developed specifically for the study helium and can not be easily generalized to the case of the heavy multi-electron atoms) the definite advantage of the presented approach. In Table 2 we present the resonance energies and widths for the 2p3s,2p3p resonances in the beryllium spectrum.

Table 2

The energy position E, width Γof the Be 2p3s, 2p3p resonances (see text)

nl	Exp, WLB	Exp, (EMR) (ME)	Th, TSB	Th, CHC	Th, KTZM	Our data
3s	10.889	10.93 10.71	10.915	10.63	10.910	10.903
3p	531(10)	-	606	-	473	478

The experimental (by Wehlitz-Lukic-Bluett, WLB; by Mehlman-Balloffet-Esteva, ME; by Esteva-Mehlman-Balloffet-Romand, EMR) and alternative theoretical data by Chi-Huang- Cheng (CHC), Tully-Seaton-Berrington (TSB) and by Kim- Tayal-Zhou-Manson (KTZM) are taken from Ref. [4].In whole a detailed analysis shows quite physically reasonable agreement between the presented theoretical and experimental results. But some difference, in our opinion, can be explained by different accuracy of estimates of the radial integrals, using the different type basis's (different degree of the gauge invariance performance), degree of accounting for the exchange-correlation effects and some other additional computing approximations.

References

1. Smirnov A.V., Buyadzhi V.V., Ignatenko A.V., Glushkov A.V., Svinarenko A.A., Spectroscopy of the complex autoionization resonances in spectrum of beryllium// Photoelectronics.-2016.-Vol.25.-P.26-33.
2. Glushkov A., Svinarenko A., Ternovsky V., Smirnov A.V. , Zaichko P., Spectroscopy of the complex autoionization resonances in spectrum of helium: Test and new spectral data// Photoelectronics .-2015.-Vol.24.-P.94-102.
3. Luc Koenig E., Aymar M., Van Leeuwen R., Ubachs W., Hogervorst W.//Phys. Rev.A.-1995.-Vol.52.-P.208-215.

4. Wehlitz R., Lukic D., Bluett J.B., Resonance parameters of autoionizing Be 2pnl states// Phys.Rev.A.-2003.-Vol.65.-P. 052708.
5. SakhoI., Konté K., Ndao A.S., Biaye M., Wagué A., Calculations of $(nl)^2$ and (3lnl') autoionizing states in two-electron systems//Phys.Scripta.-2010.-Vol.82.-P. 035301 (8pp)
6. Ho Y.K., Autoionizing $^1P^0$ states of He between the N=2,3 threshold He^+//Phys. Rev.A.- 1991.-Vol.44.-P.4154-4161.
7. Glushkov A.V., Relativistic Quantum Theory. Quantum mechanics of Atomic Systems.-Odessa: Astroprint, 2008. -700P.
8. 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, Mg-Like and Ne-Like Ions//Phys.Scripta.–1985.-Vol.32,N5.-P.513-522.
9. Ivanova E.P., Ivanov L.N., Aglitsky E.V., Modern Trends in Spectroscopy of multi-charged Ions// Phys.Rep.-1988.-Vol.166,N6.-P.315-390.
10. Glushkov A.V., Ivanov L.N., Ivanova E.P., Radiation decay of atomic states. Generalized energy approach// Autoionization Phenomena in Atoms.- M.: Moscow State University.-1986. –P.58-160.
11. Glushkov A.V., Ivanov L.N., Radiation decay of atomic states: atomic residue polarization and gauge noninvariant contributions//Phys.Lett.A.-1992.-Vol. 170, N1.-P.33-36.
12. Ivanov L.N., Ivanova E.P., Knight L., Energy approach to consistent QED theory for calculation of electron-collision strengths// Phys. Rev.A.-1993.-Vol. 48.-P.4365-4374.
13. Glushkov A.V., Khetselius O.Yu., Svinarenko A.A., Relativistic theory of cooperative muon-gamma-nuclear processes: Negative muon capture and metastable nucleus discharge// Advances in the Theory of Quantum Systems in Chemistry and Physics (Springer).-2012.-Vol.22.-P.51-68.
14. 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 (Springer).-2008.-Vol.18.-P.543-560.
15. Glushkov A.V., Svinarenko A.A., Ignatenko A.V., Spectroscopy of autoionization resonances in spectra of the lanthanides atoms// Photoelectronics.-2011.-Vol.20.-P. 90-94.
16. Svinarenko A.A., Nikola L.V., Prepelitsa G.P., Tkach T., Mischenko E., The Auger (autoionization) decay of excited states in spectra of multicharged ions: Relativistic theory//Spectral Lines Shape.-2010.-Vol.16.-P.94-98
17. Svinarenko A.A., Spectroscopy of autoionization resonances in spectra of barium: New spectral data // Phototelectronics.-2014.-Vol.23.-P.85-90.
18. Malinovskaya S V, Glushkov A V, Khetselius O Yu, Svinarenko A A, Mischenko E.V., Florko T.A., Optimized perturbation theory scheme for calculating the interatomic potentials and hyperfine lines shift for heavy atoms in the buffer inert gas//Int. Journ.of Quantum Chemistry.-2009.-Vol.109, Issue 14.-P.3325-3329.
19. Glushkov A V, Ambrosov S V, Loboda A V, Chernyakova Yu, Svinarenko A A , Khetselius O Yu, QED calculation of the superheavy elements ions: energy levels, radiative corrections, and hfs for different nuclear models//Journal Nucl. Phys. A.: nucl. and hadr. Phys.-2004.-Vol.734.-P.21
20. 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 (Springer).-2008.-Vol.18.-P.525-541.
21. Khetselius O.Yu., Relativistic perturbation theory calculation of the hyperfine

structure parameters for some heavy-element isotopes//Int. Journ. of Quantum Chemistry.-2009.-Vol.109, Issue 14.-P.3330-3335.
22. Glushkov A V, Ivanov L N, DC Strong Field Stark Effect for Non-hydrogenic Atoms: Consistent Quantum Mechanical Approach // Journal of Physics B: Atomic, Molecular and Optical Phys.-1993.-Vol.26,N14.-P.L379 – L386.
23. Glushkov A.V., Relativistic and correlation effects in spectra of atomic systems.-Odessa: Astroprint.-2006.-400P.
24. Glushkov A.V., Atom in electromagnetic field.-Kiev: KNT, 2005.
25. 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.
26. 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.
27. 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.
28. 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.
29. Glushkov A.V., Svinarenko A.A., Khetselius O.Yu., Buyadzhi V.V., Florko T.A., Shakhman A.N., Relativistic Quantum Chemistry: Advanced approach to construction of the Green's 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.
30. 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.Brändas, G.Delgado-Barrio (Springer).-2015-Vol.29.-P.55-76.
31. 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.
32. 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.
33. 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.217-229.
34. Malinovskaya S.V., Glushkov A.V., Khetselius O.Yu., Svinarenko A., Bakunina E.V., Florko T.A., The optimized perturbation theory scheme for calculating interatomic potentials

and hyperfine lines shift for heavy atoms in buffer inert gas//Int. Journ.of Quantum Chemistry.-2009.-Vol.109.-P.3325-3329.
35. Khetselius O.Yu., Relativistic perturbation theory calculation of the hyperfine structure parameters for some heavy-element isotopes//Int. Journ. of Quantum Chemistry.-2009.-Vol.109,N14.-P.3330-3335.
36. Glushkov A.V., Svinarenko A.A., Khetselius O.Y., Buyadzhi V.V., Florko T.A., Shakhman A., 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 Chemistry and Physics.-2015.-Vol.29.-P.197-217.
37. Ternovsky V.B., Glushkov A.V., Zaichko P., 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.
38. 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.
39. Glushkov A.V., Mansarliysky V.F., Khetselius O.Yu., Ignatenko A.V., Smirnov A., Prepelitsa G., Collisional shift of hyperfine line for thallium in an atmosphere of the buffer inert gas//J. Phys.: Conf. Ser. (IOP).-2017.-Vol.810.-P. 012034.
40. Buyadzhi V.V., Zaichko P.A., Gurskaya M., Kuznetsova A.A., Ponomarenko E.L., Ternovsky E.,Relativistic theory of excitation and ionization of Rydberg atoms in a Black-body radiation field//J. Phys.: Conf. Series.-2017.-Vol.810.-P. 012047.
41. Ivanova E P, Glushkov A V, Theoretical investigation of spectra of multicharged ions of F-like and Ne-like isoelectronic sequences// Journal of Quantitative Spectroscopy and Radiative Transfer.-1986.-Vol.36, Issue 2.-P. 127-145.
42. 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.
43. 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.
44. 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.
45. 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.
46. 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.
47. Khetselius O.Yu., Hyperfine structure of atomic spectra.-Odessa: Astroprint, 2008.-210P.
48. Khetselius O.Yu., Hyperfine structure of radium// Photoelectronics.-2005.-N14.-P.83-85.
49. Khetselius O., Spectroscopy of cooperative electron-gamma-nuclear processes in heavy atoms: NEET effect// J. Phys.:

Conf. Ser.-2012.- Vol.397.-P.012012
50. 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.
51. 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.
52. 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.
53. Glushkov A V, Malinovskaya S V, Gurnitskaya E P, Khetselius O Yu, Dubrovskaya Yu V, Consistent quantum theory of recoil induced excitation and ionization in atoms during capture of neutron// Journal of Physics: Conf. Series (IOP).-2006.-Vol.35.-P.425-430.
54. Glushkov A.V., Khetselius O.Y., Brusentseva S.V., Zaichko P.A., Ternovsky V.B., Studying interaction dynamics of chaotic systems within a non-linear prediction method: application to neurophysiology// Advances in Neural Networks, Fuzzy Systems and Artificial Intelligence, Ser: Recent Adv. in Computer Engineering, Ed. J.Balicki.-2014.-Vol.21.-P.69-75.
55. 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.
56. Khetselius O Yu, Relativistic calculation of the hyperfine structure parameters for heavy elements and laser detection of the heavy isotopes// Phys. Scripta.-2009.-Vol.T135.-P. 014023.
57. Glushkov A.V., Khetselius O.Yu., Gurnitskaya E.P., Loboda A.V., Florko T.A., Sukharev D.E., Lovett L., Gauge-Invariant QED Perturbation Theory Approach to Calculating Nuclear Electric Quadrupole Moments, Hyperfine Structure Constants for Heavy Atoms and Ions//Frontiers in Quantum Systems in Chemistry and Physics, Series: Progress in Theoretical Chemistry and Physics (Springer), 2008.-Vol.18.-P.507-524.
58. Glushkov A.V., Ambrosov S.V., Loboda A.V., Gurnitskaya E.P., Prepelitsa G.P., Consistent QED approach to calculation of electron-collision excitation cross sections and strengths: Ne-like ions// Int. Journal Quantum Chem.-2005.-Vol.104, Issue 4.-P.562–569.
59. 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, Issue 1.-P.195-204.
60. Glushkov A.V., Ambrosov S.V., Ignatenko A.V., Korchevsky D.A., DC Strong Field Stark Effect for nonhydrogenic Atoms: Consistent Quantum Mechanical Approach // Int. Journ. Quant. Chem.-2004.-Vol.99,N6.-P.936-939.
61. 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.
62. 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.
63. 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.
64. 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.
65. Khetselius O.Yu., Hyperfine structure of energy levels for isotopes 73Ge, 75As, 201Hg// Photoelectronics.-2007.-N16.-P.129-132.
66. 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.
67. Glushkov A.V., Svinarenko A.A., Buyadzhi V.V., Zaichko P., Ternovsky V., Chaos-geometric attractor and quantum neural networks approach to simulation chaotic evolutionary dynamics during perception process// Advances in Neural Networks, Fuzzy Systems and Artificial Intelligence, Series: Recent Advances in Computer Engineering, Ed. J.Balicki.-2014.-Vol.21.-P.143-150.
68. Glushkov A.V.,Malinovskaya S.V., Chernyakova Yu.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.
69. Glushkov A V, Negative ions of inert gases// JETP Lett.-1992.-Vol.55, Issue 2.-P.97-100.
70. 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.
71. 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.
72. 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.
73. Glushkov A.V., Energy Approach to Resonance states of compound superheavy nucleus and EPPP in heavy nuclei collisions// Low Energy Antiproton Phys. AIP Conference Proceedings.-2005.-Vol.796 (1).-P.206-210.
74. 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.

UDC 539.183

A. V. Smirnov, O. Yu. Khetselius, V. V. Buyadzhi, A. S. Belodonov

ADVANCED RELATIVISTIC APPROACH IN SPECTROSCOPY OF COMPLEX AUTOIONIZATION RESONANCES IN ATOMIC SPECTRA

Abstract

We present an advanced relativistic approach to to studying autoionization resonances parameters in the atomic systems, which is based on an generalized energy approach (Gell-Mann and Low S-matrix formalism) combined with the relativistic multi-quasiparticle perturbation theory with the Dirac-Kohn-Sham zeroth approximation and accurate accounting for the exchange-correlation, relativistic corrections. The optimization of relativistic orbitals base is reduced to minimization of the gauge dependent multielectron contribution of the lowest QED PT corrections to the radiation widths of atomic levels, which in their turn leads to the Dirac-Kohn-Sham-like equations for the electron

density. As illustration of an advanced approach application there are presented the results on energy and width for the autoionization resonance 3s3p $^1P_0$ in helium He atom spectrum, namely, the available experimental data and those results of other theories, including, method of complex rotation by Ho, algebraic approach by Wakid-Callaway, diagonalization method by Senashenko-Wague etc.

Key words: spectroscopy of autoionization resonances, advanced relativistic approach, helium

УДК 539.183

А. В. Смирнов, О. Ю. Хецелиус, В. В. Буяджи, А. С. Белодонов

УСОВЕРШЕНСТВОВАННЫЙ РЕЛЯТИВИСТСКИЙ ПОДХОД В СПЕКТРОСКОПИИ СЛОЖНЫХ АВТОИОНИЗАЦИОННЫХ РЕЗОНАНСОВ В АТОМНЫХ СПЕКТРАХ

Резюме

В работе развивается усовершенствованный релятивистский подход к изучению параметров автоионизационных резонансов в атомных системах, который основывается на обобщенном энергетическом подходе (S-матричный формализм Гелл-Манна и Лоу) и релятивистской многочастичной теорией возмущений с нулевым приближением Дирака-Кона-Шэма и аккуратным учетом обменно-корреляционных, релятивистских эффектов. Оптимизация базиса релятивистских орбиталей сводится к минимизации калибровочно-зависимого многоэлектронного вклада от обменно-корреляционных поправок КЭД теории возмущений в радиационные ширины атомных уровней, что в свою очередь, сводится к решению системы уравнений типа Дирака-Кона-Шэма для электронной плотности. В качестве иллюстрации возможностей предлагаемого подхода приведены данные по энергии и ширине автоионизационного резонанса 3s3p $^1P_0$ в спектре атома гелия и проведено сравнение с имеющимися экспериментальными данными и результатами других теорий, в том числе, методом комплексного вращения Хо алгебраического подхода Wakid-Callaway, метода диагонализации Senashenko-Wague и т.д.

Ключевые слова: спектроскопия автоионизационных резонансов, усовершенствованный релятивистский подход, гелий

УДК 539.183

А. В. Смірнов О. Ю. Хецеліус, В. В. Буяджи, О. С. Белодонов

УДОСКОНАЛЕНИЙ РЕЛЯТИВІСТСЬКИЙ ПІДХІД В СПЕКТРОСКОПІЇ СКЛАДНИХ АВТОІОНІЗАЦІЙНИХ РЕЗОНАНСІВ В АТОМНИХ СПЕКТРАХ

Резюме

В роботі розвивається вдосконалений релятивістський підхід до вивчення параметрів автоіонізаціонних резонансів в атомних системах, який ґрунтується на узагальненому енергетичному підході (S-матричний формалізм Гелл-Манна і Лоу) і релятивістської багаточастинковій теорії

збурень з нульовим наближенням Дірака-Кона-Шема і акуратним урахуванням обмінно- кореляційних, релятивістських ефектів. Оптимізація базису релятивістських орбіталей зводиться до мінімізації калібрувально-залежного багатоелектронного вкладу від обмінно-кореляційних поправок КЕД теорії збурень в радіаційні ширини атомних рівнів, що в свою чергу, зводиться до вирішення системи рівнянь типу Дірака-Кона-Шема для електронної густини. В якості ілюстрації можливостей запропонованого підходу наведені дані по енергії і ширині автоіонізаційного резонансу $3s3p\ ^1P_0$ в спектрі атома гелію і проведено порівняння з наявними експериментальними даними і результатами інших теорій, в тому числі, методом комплексного обертання Хо, алгебраїчного підходу Wakid-Callaway, методу діагоналізації Senashenko-Wague і т.і.

Ключові слова: спектроскопія автоіонізаційних резонансів, удосконалений релятивістський підхід, гелій

UDC 621.315.592

N. S. Simanovych, Ye. V. Brytavskyi, M. I. Kutalova, V. A. Borshchak, Y. N. Karakis

Odessa I. I. Mechnikov National University, 42, Pastera Str; phone: 723-34-61
e-mail: ndl_lepikh@gmail.com.ua.

THE STUDY OF HETEROGENEOUS SENSITIZED CRYSTALS OF CADMIUM SULFIDE. PART I ABOUT CHARGE OF THE CENTERS RECOMBINATION

The photovoltaic properties of CdS crystals with combined alloying have been investigated. An analytical expression for the dependence of the coefficient of damping of the intensities of exciting and quenching light has been received. For the first time the concentration of fast recombination centers has been estimated.

Charge status of S- and R-centers has been calculated. At the same time an exclusive method of solving the system of equations was created. Modulation of illumination-current characteristics with infrared light has been demonstrated.

Sensitization of semiconductors can be observed in that case if in the crystal, which already has effective centers of recombination, enter the same effective traps for carriers of one of the characters, preferably minor. Then, upon photoexcitation, due to the shortage of appropriate media, the rate of recombination is significantly reduced and the photocurrent is increasing.

This effect was first theoretically developed in the monograph A. Rose, by example, of cadmium sulfide. With well-chosen parameters, according to calculations of the author, the lifetime of the main carriers could grow up to five orders of magnitude. The concentration of recombination and sensitized centers ~ 10^{15} cm^{-3} was used. They are named respectively the 1st and 2nd classes. The magnitude of the capture cross section for electrons and holes was taken to be equal

$$S_{1n} = S_{1p} = S_{2p} = 10^{-16}\,sm^2\ ;$$
$$S_{2n} = 10^{-21} sm^2 \qquad (1.1)$$

The centers of the first class R. Bube called fast or S-centers ("Speed"), and the centers of the second class, respectively slow, due to the strongly different capture cross section, or R-centers ("Recombination"). In the present work, all three designations (class 1, fast, S-centers) will be used as synonyms.

The simultaneous existence in the sample of the fast and slow centers in detectable concentrations creates the conditions for effect, reversed to sensitizing, named infrared (IR) – absorption photocurrent. Upon excitation of such a crystal with its own light, and then with the IR illumination, the photocurrent may be reduced. This is due to the release of IR photons captured at the centers of the 2nd class cavities with the corresponding enhancement of the recombination of majority carriers. To estimate the damping was introduced the ratio Q which is equal to the change of the photocurrent relatively to the original values.

It should be noted that because it is determined not the current, and its relative (including little) change, significantly increases the sensitivity of the method to external influences (light, temperature, voltage). At the same time decreases the influence of unavoidable noise. Secondly, due to the peculiarities of alloying it is possible to create a single-chip sensors of different wavelengths, whereas for the own conductivity of the semiconductor it is not possible. Finally, while it is easily possible to create a spatially inhomogeneous sensitive system, it is not feasible on the basis of isotropic crystals.

Therefore, we chose the effect of infrared quenching of photocurrent as a research tool. In our opinion, this approach has several advantages.

First of all, if the investigated crystals sufficiently saturated with S - and R - centers, the distance between them is small. In this case, holes, embossed by IR light from the centers of slow

recombination, after only a few broadcasts of the crystal lattice passed, will be taken to S-centers and immediately affect on the value of the flowing current. Moreover, if the S - and R-centers are distributed uniformly, the path length will be more or less standardized. In a typical situation, these processes are disguised with a scattering, accidental captures in traps, unauthorized channels of recombination, etc.

In addition, the specificity of IR-quenching allows to independently manipulate both parameters current forming their own light, and the intensity and spectral distribution of infrared light, solely responsible for the release of holes. The possibilities of infrared quenching allows to selectively use the light in certain wavelengths instead of the whole spectrum.

Finally, the effect of IR-quenching allows to highlight and to explore the mechanism of emission of carriers from one particular class of centers, whereas in the usual case we have to deal with a whole range of traps, the process of devastation which camouflage each other.

These features of the infrared blanking make it a sensitive and flexible method of studying the intricacies of the photoexcitation of the non-native speakers. In addition, the combined effects of the crystals allowsthe parametric control of the processes.

As a support of the semiconductor research was selected semiconductor single crystal cadmium sulfide. Its advantages are: firstly, high photosensitivity (fotoresponseis up to seven orders of magnitude) and comparative ease of application of electrical contacts and a significant coefficient of solubility for most legants. Secondly, the presence of sensitivized R-centers, which is typical for a relatively narrow class of substances. Finally, thirdly, it is a wide bandgap semiconductor (E_g~2,42 eV), that allowed to carry out research in a wide range of wavelengths from 400 to 1600 nm with well-separated four sections – surface, own, trapping of absorption and IR spectra. In some cases, such crystals are convenient to use as a model material.

The high sensitivity of cadmium sulfide accounts for 520 nm and corresponds well to the solar spectrum. This allows to use it not only in the laboratory but also under natural light to create sensors for various purposes.

The aim of this work is the study based on the effect of IR-quenching of photocurrent of the nuances of the processes occurring upon excitation of charge carriers from the bound in the conductive state in the crystals of cadmium sulfide with an unevenly distributed impurities.

1.1. The dependence of the infrared quenching from intensities of exciting and quenching light

The concentration of free carriers normally is expressed in the population of recombination centers of 1st and 2nd classes, which themselves vary at different levels of the exciting and quenching light. This considerably complicates the calculations, making them less accurate and, in fact, not acceptable in practice. The expression for the explicit form of $Q(L_e;L_q)$ in the literature we could not find.

While illuminating the crystals only with its own light with intensity L_e the concentration of free electrons n (e) (when the absorption coefficient α and light of its own quantum output β) is given by

$$n(в) = \alpha \beta L_e \tau_{n1.} \qquad (1.2)$$

In (1.2) taken into account that the recombination is carried out mainly through the S-centers and, consequently, the life-time τ_{n1} is determined by this channel.

At sufficiently high intensities of the exciting light value τ_{n1} does not depend on its intensity, since the difference between the concentrations of free carriers (n–p), is equal to the change in the filling of recombination centers, is much less than the concentration of these centers. So on the chart of lux-ampere characteristics (LAC)is observed two sections with different slopes at high and low intensities of exciting light (tab at Fig. 1.1).

The change of formation mechanism of the photocurrent and, accordingly, the slope of a plot of LAC occurs when the number of incident photons becomes comparable with the concentration of recombination centers. This is due to the ratio

of the concentration of incident photons and fast recombination centers. When the light intensity is small, the number of absorbed photons, and hence the number of exempt carriers is less than the concentration of fast recombination centers. In this situation they can effectively contribute to the recombination of electrons and holes. For a large light fluxes, the number of photoexcited carriers is larger than the number of centers where they could recombine. S-centers can not cope with increasing concentration of free electrons and holes and the recombination rate is limited only by the throughput capacity of the centers, regardless of the total number of carriers. The situation is stabilizing. If so, then the inflection point on the LAC (in our case L_{0e} = 3,2 lx) can be estimated by order of magnitude the concentration of S-centers.

The mechanical equivalent of light A = 0.0016 and a photon energy equal to the width of forbidden zone of CdS E_g = 2,42 eV, we obtain the number of photons $N_f = L_{0e}/E_g$ = of $2.88 \cdot 10^{17}$ s^{-1} m^{-2} in the used light flux. In a typical specimen dimensions 1x1x1,2 mm from this thread on its front surface we have $N_f = 3{,}46 \cdot 10^{11}$ s^{-1} of photons. They are all absorbed in the crystal volume of $1.2 \cdot 10^{-3}$ sm^3. Therefore, the volume concentration of the recombination centers N_r is equal to the number of photons evenly distributed in this volume, will be $N_r = 2{,}88 \cdot 10^{14}$ sm^{-3}. The obtained value of $3 \cdot 10^{14}$ sm^{-3} [1,2,3], we consider as the lower limit of the doping impurity recombination. Because of the capture cross section for holes at the centers of the 1st and 2nd classes differs by five orders of magnitude, then about as many different of rates of recombination on them. Therefore, it can be argued that the value almost entirely refers to the concentration of fast recombination centers. Note that this value Rose A. operates without any justification.

The proposed method is innovative. Up to the present time for S-centers was determined with cross-section grips and, with certain reservations, the energy of activation. In any case, the zone charts show these levels closer to the conduction band. The question of their concentrations remained open.

When you turn on infrared light with corresponding energy redistribution of the holes occurs, and hence the rate of recombination through the centers of I-st and II-d class changes. Recombination throw the R - centers is getting even less, and throw the S - centers increases. Therefore, the formula $f = q'_{n1}$ remains valid.

In each act of recombination interacts with one carrier of both signs, so the rate of recombination of electrons and holes to the same level are equal $q'_{n1} = q'_{p1}$. Then you can write

$$f = q'_{p1} \ , \tag{1.3}$$

where

$$q'_{p1} = \frac{p + \partial p}{\tau_{n1}} \tag{1.4}$$

It is considered that under the action of infrared light, the concentration of holes at the centers of the second class decreased with ∂P and increased respectively at the same concentration of holes in the valence band.

If in the unit of time the quantum of quenching light L_q drops on the crystal, then in unit of volume will be absorbed $\alpha' \cdot L_q$ quantums, where α' - is the fraction of the slow recombination centers which was interected with light. Hence the additive in the concentration of free holes

$$\partial p = \alpha' \cdot L_q \cdot \tau_{P0} \ , \tag{1.5}$$

where τ_{p0}- is the lifetime of free carriers. Since the recombination of the holes also is mainly carried out through the S - centers, use

$$\partial p = \alpha' \cdot L_q \tau_{P1} \tag{1.6}$$

For large excitation level with its own light p=n and the expression (1.3) with (1.4) and (1.5) takes the form

$$\alpha \cdot L_e = \frac{n}{\tau_{p1}} + \alpha' \cdot L_q \tag{1.7}$$

$$n_{(g,q)} = \left(\alpha \cdot L_e - \alpha' \cdot L_q\right) \cdot \tau_{p1} \tag{1.8}$$

Formula (1.8) describes the dependence of the concentration of free electrons from the concurrent intensities of exciting and quenching light.

If the intensity of infrared light is not very big, then $\partial p < p_{r2}$. Population density in the holes of

the R-centers does not change very much, and the value τ_{p1} does not depend from the infrared light.

Expressions (1.2) and (1.8) allow to obtain the dependence of IR-quenching from intensities of used light fluxes [4]:

$$Q = \frac{I_{f(e)} - I_{f(e,q)}}{I_{f(e)}} = \frac{n_{(e)} - n_{(e,q)}}{n_{(e)}} = \frac{\alpha \cdot L_e \cdot \tau_{n1} - (\alpha \cdot Le - \alpha' \cdot Lq) \cdot \tau_{p1}}{\alpha \cdot Le \cdot \tau_{n1}}$$

or after transformations:

$$Q(L_q; L_e) = \left[\left(1 - \frac{\tau_{p1}}{\tau_{n1}} \right) + \frac{L_q}{L_e} \cdot \left(\frac{\alpha}{\alpha'} \cdot \frac{\tau_{p1}}{\tau_{n2}} \right) \right] \cdot 100\% \quad (1.9)$$

Formula (1.9) shows the dependence of the optical quenching from the intensities of exciting and quenching light. It should be noted that this relation is valid for small intensities of quenching light and for high levels of photoexcitation, when you can not take into account the change of populations of recombination centers.

The total experimental results of the behavior of the coefficient of quenching Q with the change of quantities of the light fluxes are shown at Fig. 1.1.

As a reference for them to take the curve 2, measured at the same intensities of its own and quenching lights, as in the case 1.1a and case 1.1b. On the left part of figure 1.1a, is shown how the value changes upon variation of the excitation light at a constant quenching. At Fig.1.1b, on the contrary, a reference curve was fixed the intensity of the excitation light and was changing of quenching light.

All graphs on Fig.1.1 received in steady-state conditions. In each point was kept sufficiently long relaxation (up to 20 minutes) to avoid the processes described in [5,6,7]. Relaxation characteristics of crystals will be discussed in part II.

First of all, note that any combinations of the intensities of short-wave maximum (Fig.1.1) was far below than long-wave [3,8]. This is due to thermal swap for the captured carriers. Due to the absorption of the phonon, one part of the holes from basic R-level moves to an excited R'. And the population of these levels with holes identifies relevant peaks. For this reason, as can be seen from figures (1.1a, b), to changes in the intensities of each light, the more sensitive is the first maximum (short-wave).

As can be seen from Fig. 1.1b, the smaller the intensity of the quenching light, L_e = *const* the smaller is the value Q . Moreover, for smaller intensities of the self-excitation it was manifested brighter. Experimentally was managed to create a situation when shortwave maximum disappeared completely [9,10].

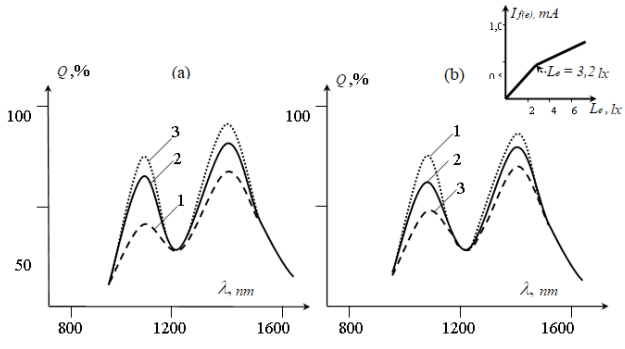


Fig. 1.1. The dependence of the value of quenching from the intensities of used light. a) L_q = const, $L_{e1} > L_{e2} > L_{e3}$; b) L_e = const , $L_{q1} > L_{q2} > L_{q3}$ .The experimental points are not plotted in order not to clutter the drawing.

At the same time, with the same intensity of quenching light (see Fig.1.1 a), with decreasing excitation L_e, the value of the coefficient of quenching increases. Moreover, this increase we saw more if used intensities L_q were negligible.

These experimental behaviors Q (L_e; L_q) confirm the validity of formula (1.9).

1.2. Critical modes of lighting crystals with infrared quenching of photocurrent

Formula (1.9) shows the dependence of the optical quenching from the intensities of exciting L_e and quenching light L_q. It should be noted that this relation is valid for relatively low intensities of quenching light and high levels of photoexcitation, when you can not take into account the change of populations of recombination centers.

As a rule, if the effect of the quenching of the photocurrent is clearly distinguishable, in all combinations of the intensities the short-wave maximum quenching (1080-1100 nm) was far below that long-wave (1380-1400 nm). This is due to thermal swap for the captured carriers. Due to the absorption of phonons, the part of

holes from the basic R-level, moves to an excited R' (discussed in part III). And the population of these levels with holes identifies the relevant peaks. For this reason, for the changes of the intensities of each light the more sensitive is the first maximum (high).

Among the restrictions imposed in the derivation of formula (1.9), was that all holes, embossed by light levels R – R' remain in the valence band and enhance the capture on S-centers. Generally speaking, this is incorrect. The capture of cross section of holes S - and R-centers are equal. However, just photoexited hole spatially is near R-centre and probably will be again captured [8]. Similar, probably multiple, oscillations did not occur at fixed external parameters and lead to useless absorption of photons of infrared light. It is obvious that this process can camouflage the dependence of the intensity of the infrared light. More this effect will be discussed in part II.

Under the critical light levels, as exciting and quenching light, we will understand these light beams, when on the spectral distribution of coefficient of quenching are not only mentioned in section 1.1 quantitative change, but there is a quality changes[10].

As was noted above that because of the growth of intensity of self-excitation and reducing of the flow of infrared radiation the value of quenching in accordance with the formula (1.9) decreases. When a critical ratio of these intensities, it is possible when on the curve of spectral distribution $Q(\lambda)$ completely disappears shortwave maximum, then the long-wave still is present. Formula (1.9) for this case is not applicable because violation of tolerance limits aremade at its conclusion.

The processes in this case can be explained as follows. The smaller the value L_q, the less infrared photons knock out holes from R-centers. Accordingly, fewer of them come to the fast recombination centers and the decline of majority carriers – electrons becomes less. It is this relative reduction estimates (using current) the value of the coefficient Q. The greater the intensity of its own light and, accordingly, the initial concentration of free electrons, the less is noticeable their decrease in recombination. First and foremost, from graphic is disappearing shortwave maximum $Q(\lambda)$, as it relates to the liberation of holes from the basic state of R-centers, where the concentration of charge is less because of thermal pumping to R'- states.

The reverse situation (see Fig. 1.2) – maximum flow of infrared light and extremely high levels of self-photoexcitation – we observed not previously described in the literature, the phenomenon of the disappearance of the long-wave maximum quenching of the photocurrent (1380 – 1400 nm), whereas shortwave maximum $Q(\lambda)$ in the region of 1080 – 1100 nm was still remained.

The limit levels of exposure were determined by the capabilities of the experimental unit. In the area of maximum photosensitivity of the sample (520 – 530 nm) intensity of monochromatic light provided the illumination of order 5 – 6 lx.

In our case, the determining impact provide the mechanisms of formation of maximums $Q(\lambda)$ by themselves. For the reasons that were described above, due to the redistribution of the concentration of trapped holes, the shortwave maximum of quenching (~ 1100 nm) lower than the wavelength must to disappear first in suboptimal ratio of the intensities of clipping.

Abnormal view of curve $Q(\lambda)$ with a missing long-wavelength maximum (~ 1380 nm), we explain in the following way. In accordance with the formula (1.9) the value of coefficient Q does not depend on the intensity L_q and on result $L_q\beta'$, including the value of the quantum yield. The authors [3] have noted that for some ratios of intensities of light fluxes, the magnitude of the quantum yield for infrared radiation in the samples with R-centers can quickly decrease. Experimentally were recorded the values of the order $\beta'=0{,}026\div0{,}072$ [8]. At such small values the decrease of β' can be decisive even at relatively high values of L_q in the numerator of (1.9).

To explain the dependence of $Q(\lambda)$ for this case we propose the following mechanism. When we are illuminating by light with a wavelength corresponding to the activation energy of R' - centers, the number of seats available to them increases. In this case the outflow of thermally excited holes from R-levels should increase. In turn, this leads to an increasing of seats available at those levels. As a result, the repeated captures of holes to R' centers are increasing, and the quantum yield for infrared radiation is even lower.

Note that the described effect, obviously, can be carried out for each set temperature only in a narrow range of ratios between the existing concentration of R-centers and used its own intensity of light and infrared radiation. Analysis is easier to carry out under the condition when only the intensity of light of its own relatively changes according to the other three fixed parameters.

If your exiting is too great, in the *V*-zone is a large number of free holes. Additional charge, embossed by IR-radiation from R-centers, can not significantly change their concentration, and thus the flowing current.

Besides, R-centers are heavily populated by holes (probably, even $p_r \approx N_r$; $p_{r'} \approx N_{r'}$). Relatively small changes caused by IR photons are not able to affect the existing ratio of concentration of the charges on the centers. Moreover, the resulting empty spaces will be filled with holes from the valence band.

On the contrary, if the intensity of its own light is not large enough concentration of localized holes at the centers of class II will be lowal. In this case, before the activation of the IR light on the R-centers are a significant number of places with blank holes. The appearance of IR excitation can not make any noticeable changes in their number, and hence the balance of processes of capture-emptying.

Held arguments correspond to movement along the line AB schematic figure 2. Area 1 at Fig. 1.2 is the magnitude of the intensities when the standard mechanism of A.Roseis. In such conditions were starred family of graphs $Q(\lambda)$ Fig.1.1, and such light fluxes obtained formula (1.9).

Its output was simplify by demanding conditions $L_q \uparrow > L_e \uparrow$[4], i.e. when a significant number of photons as their own get on the sample, and infrared light, and quenching - more. For this reason, in region 2 Fig.1.2 the formula (1.9) are not applicable.

The effect of quenching may not be implemented here immediately for three reasons:

I. First, when there is small own excitation ($L_e \rightarrow 0$) the number of pairs of free nonequilibrium carriers is less than can recombine via S-centers;

II. Second, minor activation of holes from R-centers ($L_q \rightarrow 0$) is almost completely masked by the processes of dissipation, captures in traps, etc. These holes practically do not reach S centers;

III. Finally, the small number of extra holes that reach the centers of quick recombination, causing a slight decline of majority carriers – electrons – and, therefore, virtually do not impact on the change of the photocurrent.

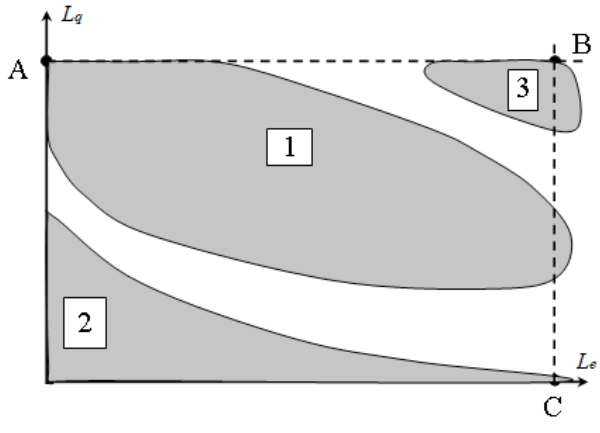


Fig. 1.2.Field of possible ratio of the intensities of exciting and quenching light; 1 – region of existence of the effect of IR-quenching of photocurrent; 2 – the area of intensity when extinction does not occur; 3 – area where you may watch the abnormal effect of quenching. Unpainted areas are transitional between these regions.

For completeness, we will hold the consideration in which area 3 Fig. 1.2 can be accessed along the line CB. That is, when extremely high level of self-excitation is recorded and the infrared flow gradually increases.

For small values of L_q quenching does not occur in virtue of the third condition for region 2. When averages L_q quenching although appears, but slightly. This corresponds to the limit situation of the region 1 Fig 1.2. Finally, for large intensities, comes into force the mechanism of the anomalous absorption, described above.

The maximums of quenching dependence $Q(\lambda)$ behave differently. The short wavelength peak in the 1100 nm may increase at the expense of complete emptying of the ground state of R-centers. Long-waved infrared (1400 nm region) can not appear even under these conditions because of the low value of quantum yield. Photoexited ones from R'-states of the hole remain in the area

of R-centers at the expense of repeated seizures and does not contribute to recombination at the S-centers.

Thus, the peculiarities of interaction of infrared radiation with the centers of class II impose limitations on the applicability of the expression $Q(L_e, L_q)$, and the relative magnitude of the maxima of the extinction.

2.1. About charge state of the centers of slow and fast recombination

Model of infrared quenching of photocurrent Bube-Rose based on the existence in the crystal the recombination centers of the two classes.

R-centers are external impurity in the sample, most likely copper in the cadmium sublattice. To get to the crystal this impurity can only in the neutral charge state. If this is a trap for holes, then it has two states: neutral and positively charged after the capture of holes. It also points to the capture cross section for holes 10^{-16} sm^2. Such values of cross sections are typical up for grabs in a neutral trap.

However, the capture cross section for electron – 10^{-21} sm^2 is the usual for grabs in a repulsive center. At the moment of electron capture, the center is already charged negatively. In this case, it is the acceptor. He gave the hole and is charged negatively. For holes it is the attractive center now and should have a corresponding capture cross section ~10^{-12} sm^2, what is not observed experimentally. On the contrary, it is established that R-centers after the capture of an electron does not possess a repulsive Coulomb barrier. These are singly charged acceptors and the electron capture occurs with a neutral center.

For holes found that with decreasing temperature the possibility of internal transfer of these carriersdecreasesin the R-centers, what is very unusual to capture at the charged centre, besides having a system of intermediate states.

Thus, there is a contradiction – there are arguments that the R-centers are either in the neutral and positively charged or neutral and negatively charged, both could not be madeat the same time. We have to assume that these states alternate, with the presence of at least one intermediate stage. A simple scheme, when a neutral acceptor would give a hole, and then captured electron with the subsequent recombination of it with the new spare hole, would require that at the final stage the hole was captured on a doubly negatively charged center, what is also not observedin the experiment.

Note that it is possible that the ensemble of R-centers consists of several groups: it may be copper in the cadmium sublattice of Cu_{Cd} or negatively charged center of the silver in the cadmium sublattice Ag_{Cd}^{-}, or even a complex neutral conglomerate of charged sulfur vacancies of sulfur and cadmium $(V_S^{2+} + V_{Cd}^{2-})$.

As for the S-centers, data on their charge state do not exist to the present time. Make any reasonable assumptions based on a simple analysis of the capture cross section for electrons and holes is impossible. It is the equality of these cross sections in a model A. Rose is doing these centers an effective channel of recombination. But in this case, if in initial state, these centers were neutral, then after the hole capture, they become positively charged. With equal probability, after the capture of an electron, they acquire a negative charge.

A. Rose model does not consider the order of the carrier capture on S-centers. In literature data about the scenario of these processes is not affected. Of the characteristics of the field drift of the centers of quick recombination at a known applied voltage polarity concluded that they are positively charged. For a long time the samples were kept under conditions of the applied field. Then were measured local probe characteristics of tactile sensing. It was discovered, the enhancement of IR-quenching of photocurrent in the near-cathode region.

At the same time centers of quick recombination are attributed to the properties of electronic traps. In this case, they can be either neutral or carry a negative charge. The question remains open and requires further study.

We attempt to resolve some of these incorrectness [11].

The interaction of charge carriers with local centers in a two-level model of recombination Bube-Rose is described by the equations:

$$S_{n1} v p_1 n = S_{p1} v n_1 p \quad (2.1)$$

$$S_{n2} v p_2 n = S_{p2} v n_2 p \quad (2.2)$$

$$n = f\,\tau_n = \frac{f}{S_{n1} v p_1 + S_{n2} v p_2} \quad (2.3)$$

Here S_{ij} - are the corresponding capture cross-sections of electrons and holes at the centers of the first and second classes; p, n – concentrations of free charge; ν – speed of thermal motion; p_1, p_2, n_1, n_2 – concentrations of electrons and holes captured in the centers of fast and slow recombination, f – the intensity of the photoexcitation; τ_n - is the lifetime of the main carriers.

The first two of these equations represent the equality of the rate of capture of holes and electrons respectively in S - and R-levels, the third is the condition of non-accumulation of charge. This assumes that the sample is sufficiently high resistance, and the intensity of the light, and with it the intensity of the photoexcitation is sufficiently large. Under these conditions, concentrations, which are included in the equations (2.1)-(2.3) are non-equilibrium carriers, and the lifetime of the main carriers obeys the expression (2.3).

The number of variables in the formulas (2.1) – (2.3) can be reduced given the fact that for large photoexcitation intensities, the number of free charge carriers is comparable or higher than the concentration of recombination centers. An idle trapsare not left. Since the recombination center, by its nature, may be occupied either by an electron or a hole, then is true

$$n_1 = N_1 - p_1 \quad (2.4)$$

$$n_2 = N_2 - p_2 \quad (2.5)$$

where N_1 and N_2 – total concentration of S - and R-centers, respectively.

To solve the system of equations (2.1) – (2.5) should be closed by the condition of electroneutrality. It's kind depends on the allowed charge states of the centers of the I-st and II-d classes. There are four possible options:

If R-centers are charged **positively**, the equation of electroneutrality is representable for **positively** charged S-centers

$$n = p + p_1 + p_2\,, \quad (2.6a)$$

or for **negative** S-centers

$$n + n_1 = p + p_2 \quad (2.7)$$

Taking into account (2.4) the expression (2.7) can be rewritten as

$$n = p + p_1 + p_2 - N_1 \quad (2.6b)$$

If R-centers are charged **negatively**, the corresponding electroneutrality conditions will have the form for **positively** charged S-centers

$$n + n_2 = p + p_1, \quad (2.8)$$

for **negatively** charged S-centers

$$n + n_2 + n_1 = p. \quad (2.9)$$

Taking into account (2.4) the expression (2.8) becomes

$$n = p + p_1 + p_2 - N_2. \quad (2.6c)$$

And taking into account (2.5) and (2.6) the expression (2.9) takes the form

$$n = p + p_1 + p_2 - N_1 - N_2 \quad (2.6d)$$

For convenience, the condition of electroneutrality for all possible cases collected in table 2.1.

Without going into details of the processes, we have carried out calculations for all four systems of equations (2.6a,b,c,d) so (2.1) – (2.3) with (2.4), (2.5).

Unknown are n, p, p_1 and p_2. Since the system of four linear equations are with four unknowns, all of them have solutions, and these solutions are single-valued and unique.

The case of **negatively** charged R-centers

It was found that for **negatively** charged R-centers the studied system of equations has no positive solutions when you use the equation of

electroneutrality in the form of (2.6b) and (2.6d).

For example, when negatively charged levels of the second class and the positively charged centers of the first class, in terms of

$f = 10^{15}\,sm^{-3}s^{-1}$;$N_1^+ = N_2^- = 10^{15}\,sm^{-3}$,

the system of equations (2.1)-(2.3),(12.6d) has the solution [12]:

$n = -1{,}005 \times 10^{15}$ sm^{-3}; $p = 4{,}988 \times 10^{7}$ sm^{-3}; $p_1 = -4{,}963 \times 10^{7}$ sm^{-3}; $p_2 = -4{,}987 \times 10^{12}$ sm^{-3}.The error function (see below) in this case was F = 0,0000077.

I.e. negative concentrations appear. This means that under the current model, the centers of slow recombination of negative charge can not bear. This conclusion is in good agreement with the value of the capture cross section for holes on these centers. The question of how the value of capture cross sections for electrons form for them remains open.

Table 2.1

Four variations of the charge States of R - and S-centers

Local levels	R-centers		
	charge	+	–
S-centers	+	$n = p + p_1 + p_2$ (2.6a)	$n = p + p_1 + p_2 - N_2$ (2.8) → (2.6c)
	–	$n = p + p_1 + p_2 - N_1$ (2.7) → (2.6b)	$n = p + p_1 + p_2 - N_1 - N_2$ (2.9) → (2.6d)

Case of **positively** charged R-centers

For positively charged R-centers and **positively** charged S-centers, the working system of equations after transformation has the form:

$$np_1 = p\,(N_1 - p_1) \quad (2.10)$$
$$np_2 = Ap\,(N_2 - p_2) \quad (2.11)$$
$$B = Anp_1 + np_2 \quad (2.12)$$
$$n = p + p_1 + p_2 \quad , \quad (2.13)$$

where $A = \frac{S_{p2}}{S_{n1}} = 10^5$; $B = \frac{f}{vS_{n2}}$.In all cases the value v was equal 10^7sm/s.

Parameters in the system of equations (2.10) – (2.13) are N_1, N_2 and f. Each of these variables can take values from a wide range of numbers from 10^{12} to 10^{18}. Therefore, we used the following tactics: concentration of S-centers fixed at the level of 10^{15}sm^{-3}, regarding it as the argument value N_2has changed from 10^{14} to 10^{16} sm^{-3}. The system of equations was solved several times for different levels of photoexcitation f=10^{14}; 10^{15}; 10^{18} sm^{-3}s^{-1} (i.e. less, equal to, and a lot more than fixed concentration of fast recombination centers). The asymmetry of the spread of selected values of f with respect to N_1 is due to the fact that the original system of equations (2.1)–(2.3) is written for large levels of photoexcitation.

From equation (2.12)

$$p_2 = \frac{B}{n} - Ap_1 \ . \quad (2.14)$$

From equation (2.10)

$$p = \frac{np_1}{N_1 - p_1} \ . \quad (2.15)$$

Dividing (2.10) by (2.11) we get

$$\frac{p_1}{p_2} = \frac{N_1 - p_1}{A(N_2 - p_2)} \quad (2.16)$$

from where

$$p_2 = \frac{AN_2p_1}{N_1 + p_1(A-1)} \quad (2.17)$$

Joint solution of (2.8) and (2.5) gives

$$p_1^2A(A\text{-}1) + p_1[A(N_2 + N_1) - \frac{B}{n}(A\text{-}1)] - \frac{BN_1}{n} = 0.$$

The solution of this quadratic equation has the form

$$p_1 = \frac{-D + [D^2 + 4A(A-1)(\frac{B}{n})N_1]^{\frac{1}{2}}}{2A(A-1)} \quad (2.18)$$

in which

$$D = [A(N_2 + N_1) - \frac{B}{n}(A\text{-}1)].$$

The "–" sign before the root in (2.18) is discarded because it leads to $p_1 < 0$.

Equation (2.14),(2.15),(2.18) after substitution in (2.13) provide an equation with one unknown variable - $n(N_2)$:

$$n = \frac{n\,p_1}{N_1 - p_1} - p_1(A\text{-}1) + \frac{B}{n}, \qquad (2.19)$$

in which, for the sake of saving accounts the value of p_1 have not been painted, in accordance with the formula (2.18).

It is obvious that the resulting expressions are too cumbersome for analysis. Since after substituting for $p_1(n)$ structure of the expression (2.19) has the form $f_1(n+\frac{1}{n}) = f_2(n + \frac{1}{n})^{1/2}$, finally, one should expect the equations of at least fourth degree relative to n. Moreover, the coefficients in this equation may vary up to 15 orders of magnitude. That is the complexity of solving the given system of equations is probably the reason why such analysis was not previously done.

Us an algebraic way to solve the system of equations (2.10) – (2.13) were discarded, and instead applied such an artificial technique.

The value of n is set arbitrarily. In accordance with the equation (2.18) is determined by the value p_1. Knowing it and n, the formulas (2.14) and (2.15) are determined by the numerical value of p_2 and p. Then all four numbers are substituted in the original system of equations, and determines the error function [see (2.10) - (2.13)]

$$F = \frac{p(N_1 - p_1)}{np_1} + \frac{Ap(N_2 - p_2)}{np_2} + \frac{Anp_1 + np_2}{B} + \frac{p + p_1 + p_2}{n} - 4 \qquad (2.20)$$

Remains, fingering n, to minimize the error function. Four introduced into the formula (2.20) to the exact solution correspond to a value of F which is equal to zero.

The peculiarity of function (2.20) is that it uses not the traditional difference of the left and right parts of the corresponding equations, and the quotient of their division. This is due to the fact that in the first three equations of system (2.10) – (2.13) are the products of the concentrations. In this case, the difference of the left and right side of equation (2.13) will be much smaller (up to 15 orders of magnitude)than the remaining contributions to the error function, being at the level of machine zero. Namely, in this equation the characteristics of the charge state of the local centers are inherent. In addition, this approach eliminates the need to do the sign of the error in each of the equations. The advantage of the proposed method is in the simultaneous receipt of all the unknown quantities.

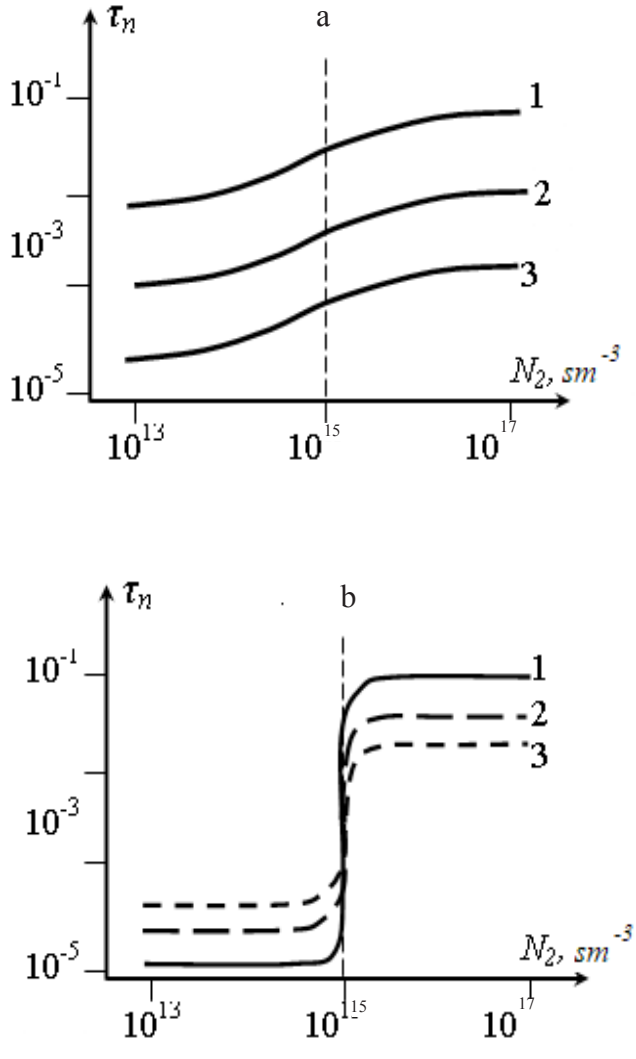


Fig. 2.1. The change of the lifetime of electrons when the concentration of R-centers for levels of photoexcitation: 1 – 10^{14} , 2 – 10^{15} and 3– 10^{17} $sm^{-3}s^{-1}$. A – the calculation was performed for positive, B - for negatively charged centers of first grade.

The value of tactile sensing, we evaluated according to the change of the lifetime of the main carriers, the value of which had counted the fill level hole centers of the I-st and II-d classes:

$$\tau_n = \frac{1}{S_{n1} p_1 v + S_{n2} p_2 v} \qquad (2.21)$$

The results of the calculations [12,13] are shown in Fig.2.1A. It is seen that if the centers of both classes are positively charged, responsivity starts at the concentration of R-centers by about two orders of magnitude below than the concentration of S-centers. Regardless of the level of photoexcitation the value of the lifetime increases by about two orders of magnitude in the case when the concentration of R-centers also increases by two orders of magnitude higher than the concentration of S-centers.

The dotted line in Fig. 2.1 shows the concentration of S-centers. As a result of the problem solution at our disposal is just as the concentration -N_1, and the concentration of holes in centers of quick recombination – p_1, it is possible to determine directly the proportion of centers that captured positive charge. Depending on the lighting conditions f and the concentration of centers N_2, value $\frac{p_1}{N_1}$ is amounted to 1-3 % . And even such S-centers in accordance with Fig. 1.1 can provide an increase in τ_n only several orders of magnitude. This is a weak and ineffective channel of tactile sensing. Nevertheless, it exists and is able to make some adjustments to the painting processes. Especially on the lower border of the governing parameters – at low levels of photoexcitation and low concentrations of the centers of the II-d-class – when the mechanism of tactile sensitizing of A. Rose (see Fig.2.1) are not yet included.

For the case of "**positively** charged R-centers – **negatively** charged S-centers" the defining system of equations in accordance with (2.10) – (2.12), (2.6d) has the form

$$np_1 = p\,(N_1 - p_1) \qquad (2.22)$$

$$np_2 = Ap\,(N_2 - p_2) \qquad (2.23)$$

$$B = Anp_1 + np_2 \qquad (2.24)$$

$$n = p + p_1 + p_2 - N_1 \qquad (2.25)$$

From equations (2.10) – (2.13) they formally differ only in the last term in the fourth equation. However, the result is thus radically different.

Note the additional difficulty posed by the fact that the area $N_2 \approx N_1$ the decision was stochastic - by changing the concentration in the second decimal place the value of lifetime was changed to five orders of magnitude (see Fig.2.1b). It had to take into account when choosing the step with which the calculations were increased and the concentration of centers of the second class.

The method of calculation was used the same as that which is described above. The results are shown at Fig. 2.1b. As experimentally quite well established, that in the sensitized cadmium sulfide lifetime of majority carriers changes by 4 – 5 orders of magnitude, from the comparison of figures 2.1a and 2.1b it follows that such a change can only be the case if the levels of the 1st class are negatively charged – are nonequilibrium electrons which are captured by neutral centers. The equation of electroneutrality is given by (2.6b).

Note that a significant sensitizing should be expected only for relatively small levels of exposure. With the increasing intensity of the photoexcitation of the upper part of the graph when $N_2 \gg N_1$ is downward sloping, whereas the lower part under the $N_2 \ll N_1$, moves towards it. As a result, the jump in the value of the lifetime after tactile sensitizing is a lot less. The effect of tactile sensitizing is concealed. This receives a natural explanation if we consider that at high rates of photoexcitation the carrier concentration is high. Introduction of the sensitized impurities of the same concentration is not able to increase it significantly.

In addition, it was found that the system of equations (2.1) – (2.3) – plus one of the conditions of electroneutrality (see table 2.1) are very sensitive to the last term in (2.6a) – (2.6d). Value when the system has physically meaningful solutions, i.e. when the principal features of the quenching appear, is about the order of 10^{15} sm^{-3}. This can be a value of concentration N_1 in the formula (2.6b) or N_2 in the formula (2.6b), or their sum $N_1 + N_2$ in the formula (2.6d) (see table 2.1). Note that the

order of magnitude was applied by A. Rose without comment. Because the description of tactile sensitizing was performed polyfermenticus and the condition of electroneutrality does not apply, there is a problem with the fetishization of that number. As a result of our consideration, was revealed the special properties of concentrations of centers of fast and slow recombination.

In the field of used values of the intensities of photoexcitation at a concentration of recombination centers is less than 10^{15} sm^{-3} tactile sensitizing does not occur at all. When this limit is reached (first column, first row of the table 2.1) sensitizing is possible, but happens only slightly (Fig.2.1a), and the number of centers which are able to participate in this process plays the decisive role. At concentrations that significantly exceed the limit of 10^{15} sm^{-3} for negative R-centers, the solution of the system of equations is formally generally falls into negative area, which has no physical meaning (second column of the table 2.1). In a narrow region on the border of these concentrations probably an avalanche-like increase of the lifetime (Fig.2.1b). But only for positively charged R-centers and negatively charged S-centers (second line, first column of the table 2.1).

The obtained results remove the existing contradictions. Properties of the S-centers are such that, while they are in the neutral state, they are able to capture an electron and a hole with the same capture cross section of 10^{-15} sm^2. As a result, the crystal are negatively and positively charged centers of the first class. However, since the material used is n-type, the mere predominance of electrons provides a more frequent seizures, and sensitizing occurs mainly according to the scenario in Fig.2.1b. The percentage ratio between the positively and negatively charged S-centers obtained for the first time. Perhaps this indicates that, analogous to a second class, the fast recombination centers also consist of several types.

2.2. Modulation of LAC type with infrared light

View of figures 2.1a and 2.1b allows to predict lux-ampere dependence for both channels, tactile sensitizing. For fixed values of concentrations of centers of N_1 and N_2 in the case when the process involves positively charged S – centers (Fig.2.1a), the increase of intensity of photoexcitation causes approximately the same decrease in the lifetime. This should facilitate the formation of a more or less linear LAC.

Similarly, for negatively charged S – centers (Fig.2.1b), after tactile sensitizing (right of dotted line), with increasing levels of photoexcitation, the lifetime was decreased. The product of these quantities $n = f \cdot \tau_n$ remains approximately the same order of magnitude. In these circumstances we should expect lux-ampere dependence is close to linear, we indeed found experimentally [4].

In the bottom of the graph Fig.2.1b, in region $N_2 \ll N_1$ when sensitizing has not yet occurred, the lifetime increases with the intensity of photoexcitation. This should result converges lux-ampere characteristic. Change the formation mechanism of the LAC is further evidence of the prevalence in the crystal's centers, which have captured negative charge in compare with positively charged.

Such change of LAC is difficult to observe in dependence on the concentration of R-centers experimentally, because you will need very similar samples with different levels of doping or single crystal with sequentially adding in an admixture. Both ways are difficult to implement. In the first case, prevents the natural spread of parameters of crystals even grown in the same batch. And the second additive doping inevitably changes the previous distribution, we introduce impurities and properties are already made by other impurities (in our case at least, the S-centers). Crystal becomes inadequate.

However, it is possible to do otherwise [12,13]. If the intensity of infrared light is such that the number of incident photons is comparable and slightly lower concentration of R-centers, the light becomes modulating. The quantum of infrared radiation, absorbed on the centers of slow recombination, is inhibit for the population of their holes. As a result of effective concentration of R-centers, which are really involved in the process of tactile sensitizing becomes less. The share of such centers for the same crystal is the smaller, the greater the intensity of IR light, which impacted the crystal.

Figure 2.2 shows a family of lux-ampere characteristics when excited by their own light (λ=520 nm) of the crystal CdS with obviously present the effect of IR-quenching of photocurrent. As the parameter, was changed the intensity of the infrared light. Since the processes of tactile sensitizing can be superimposed on the influence of excited states of R-centers, applied a multiplier range of wavelengths from 900 to 1400 nm. High light was monochromatic.

As can be seen from the figure 2.2, the effect of infrared light reduces the absolute value of the photocurrent (infrared quenching), but increases the degree of nonlinearity of the graph. For ease of comparison, the inset presents the dependence of the following values for the two extreme cases -off IR illumination (curve "a" corresponds to the curve 1 Fig.2.2) and the largest intensity of the additional infrared light (curve b corresponds to curve 3 in Fig.2.2).

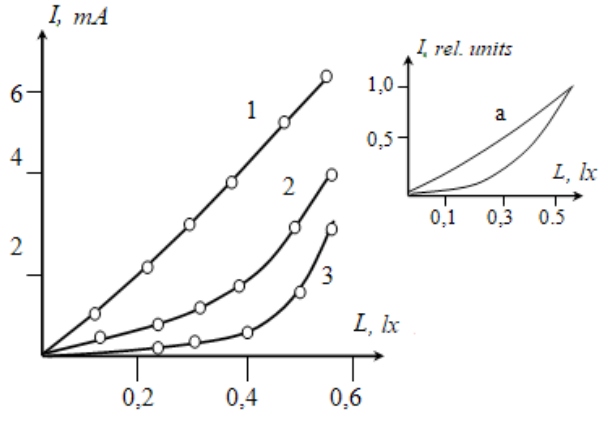


Fig. 2.2. The change of the photocurrent in the combined excitation with IR light: 1 - 0 ; 2 - 3,0·10^{-3} ; 3 - 1,4·10^{-2} lx.

As originally effect of modulation of type LAC with infrared light requires the condition $N_2 \gg N_1$, it can not be carried out for all crystals. However, if the phenomenon of the change of the lux-ampere characteristics from linear to converges which is not marked by A. Rose, after all is observed, it can serve as a good criterion of held tactile sensitizing of the sample, bypassing the estimation of the lifetime of carriers.

References

1. Новикова М.А. Особливості інфрачервоного гасіння фотоструму у напівпровідниках CdS.//Работа – лауреат Областного конкурса (1 место) Малой академии наук, Областное территориальное отделение, Секция "Физика". Одесса, 2005 г., с. 1 – 37.
2. M.A.Novikova Change of Photoelectric Properties of Semiconductors as a Tool for the Controlof Environmental Pollution by Extraneous Admixtures and IR-illumination.//Section of Environmental Science. Finalist of Intel International Science and Engineering Fair. USA, AZ, Phoenix, May 8 – 18. 2005.
3. Драгоев А.А., Затовская Н.П., Каракис Ю.Н., Куталова М.И. Управляемые электрическим полем датчики инфракрасного излучения.//Материалы 2 nd International Scientific and Technical Conference "Sensors Electronicsand Microsystems Technology" Book of abstracts. 115. Секция IV "Радіаційні, оптичні, та оптоелектричні сенсори". Україна, Одеса, 26–30 червня 2006 р. "Астропринт". 2006.
4. M.A.Novikova, Yu.N.Karakis, M.I. Kutalova Particularities of current transfer in the crystals with two types of Recombination centers. //Photoelectronics – 2005.n.14. –P. 58-61.
5. Каракис К.Ю. Релаксационные характеристики полупроводниковых кристаллов с ИК-гашением фототока.// Одесса, Работа – лауреат Областного конкурса (Ш место) Малой академии наук, Областное территориальное отделение, Секция "Физика". Одесса – 2001. с. 1–37.
6. Ю.Н. Каракис, Н.П. Затовская, В.В. Зотов, М.И., Куталова Особенности релаксации фототока в кристаллах сульфида кадмия с запорными контактами//1-а Українська наукова конференція з фізики напівпро-

відників.– Одеса, 10-14 вересня 2002. Тези доповідей. Т.2. – с.138
7. К.Ю. Каракис, В.А. Борщак, В.В. Зотов, М.М. Куталова Релаксационные характеристики кристаллов сульфида кадмия с ИК-гашением.//Фотоэлектроника 2002.– вып.11. – с.51–55.
8. A.A.Dragoev, Yu.N.Karakis, M.I. Kutalova Peculiarities in photoexcitation of carriers from deep traps.// Photoelectronics– 2006 – n. 15.–P. 54–56
9. А.А.Драгоев Визначення квантового виходу інфрачервоного гасіння фототоку.//Робота – лауреат Областної сесії Малої Академії наук України. Одеське територіальне відділення. Секція "Фізика". –Одеса 2006. – с.32 .
10. Ye.V. Brytavskyi, Yu. N. Karakis, M. I. Kutalova, G.G.Chemeresyuk Effects connected with interaction of charge carriers and R-centers basic and exited states.//Photoelectronics. –2009. –n. 18.–P. 84 – 87.
11. E.V.Britavsky, Y.N.Karakis, M.I.Kutalova, G.G.Chemeresyuk On the charge state of rapid and slow recombination centers in semiconductors//Photoelectronics.–2008. – n.17.– 2009. – n. 18–P. 65 – 69.
12. Британский Е.В. Эффект модулирования вида люксамперной характеристики инфракрасным светом //63-я отчётная студенческая научная конференция, посвящённая 143-й годовщине Одесского национального университета имени И.И. Мечникова. Физический факультет. Секция физики полупроводников и диэлектриков. 23 - 24 апреля – 2008. Тезисы докладов – С. 52 – 53.
13. G.G.Chemeresyuk, Ie. V. Brytavskyi, Yu. N. Karakis (Ukraine) Infrared radiation sensor with selective controlled sensitiviti// The Ninth International Conference "Correlation Optics 2009" – Chernivtsi National UniversityChernivtsi, Ukraine. September 20 – 24. – 2009. Poster Session. Session 2 – D-2.

This article has been received within April 2017.

UDC 621.315.592

N. S. Simanovych, Ye. V. Brytavskyi, M. I. Kutalova, V. A. Borshchak, Y. N. Karakis

THE STUDY OF HETEROGENEOUS SENSITIZED CRYSTALS OF CADMIUM SULFIDE. PART I. ABOUT CHARGE OF THE CENTERS RECOMBINATION

Summary

The photovoltaic properties of CdS crystals with combined alloying have been investigated. An analytical expression for the dependence of the coefficient of damping of the intensities of exciting and quenching light has been received. For the first time the concentration of fast recombination centers has been estimated.

The charge state of S - and R- centersis expected. The exclusive method of decision of the system of equalizations is thus created. Modulation of LAC is shown by IR light.

Key words: oefficient of damping, CdS, IR light.

УДК 621.315.592

Н. С. Сімановіч, Е. Д. Бритавський, М. І. Куталова, В. А. Борщак, Ю. М. Каракіс

ДОСЛІДЖЕННЯ НЕОДНОРІДНО ЗЧУВСТВЛЕННИХ КРИСТАЛІВ СУЛЬФІДУ КАДМІЯ. ЧАСТИНА І. ПРО ЗАРЯДОВИЙ СТАН ЦЕНТРІВ РЕКОМБІНАЦІЇ

Резюме

Досліджені фотоелектричні властивості кристалів CdS з комбінованим легуванням. Отримано аналітичний вираз для залежності коєфіціента гасіння от інтенсивностей збуджуючого і гасящего світла. Вперше оцінена концентрація центрів швидкої рекомбінації.

Розрахован зарядовий стан S- і R-центрів. При цьому створено ексклюзивний метод вирішення системи рівнянь. Продемонстрована модуляція ЛАХ інфрачервоним світлом.

Ключові слова: коєфіціент гасіння, сульфід кадмію, інфрачервоне світло.

УДК 621.315.592

Н. С. Симанович, Е. Д. Бритавский, М. И. Куталова, В. А. Борщак, Ю. Н. Каракис

ИССЛЕДОВАНИЕ НЕОДНОРОДНО ОЧУВСТВЛЁННЫХ КРИСТАЛЛОВ СУЛЬФИДА КАДМИЯ. ЧАСТЬ І. О ЗАРЯДОВОМ СОСТОЯНИИ ЦЕНТРОВ РЕКОМБИНАЦИИ

Резюме

Исследованы фотоэлектрические свойства кристаллов CdS с комбинированным легированием. Получено аналитическое выражение для зависимости коэффициента гашения от интенсивностей возбуждающего и гасящего света. Впервые оценена концентрация центров быстрой рекомбинации.

Рассчитано зарядовое состояние S- и R-центров. При этом создан эксклюзивный метод решения системы уравнений. Продемонстрирована модуляция ЛАХ инфракрасным светом.

Ключевые слова: коэффициент гашения, сульфид кадмия, инфракрасный свет.

UDC 539.182

E. V. Ternovsky, O. A. Antoshkina, T. A. Florko, T. B. Tkach

Odessa State Environmental University, L'vovskaya str.15, Odessa-16, 65016, Ukraine
e-mail: florkota@gmail.com

RELATIVISTIC CALCULATION OF OSCILLATOR STRENGTHS OF THE RADIATION TRANSITIONS BETWEEN BARIUM RYDBERG STATES

The combined relativistic energy approach and relativistic many-body perturbation theory with the zeroth order Dirac-Kohn-Sham one-particle approximation are used for preliminary estimating the energies and oscillator strengths of radiative transitions from the ground state to the low-excited and Rydberg states, in particular, 6s2 -6snp (n =7-30) transitions, of the barium atom. The comparison of the calculated oscillator strengths with available theoretical and experimental (compillated) data is performed. The important point is linked with non-accounting for the polarization effect contribution into the oscillator strength value that has led to ~40% difference between the empirical (compillated) and theoretical data.

1. Introduction

The research in many fields of modern atomic physics (spectroscopy, spectral lines theory, theory of atomic collisions etc), astrophysics, plasma physics, laser physics and quantum and photo-electronics requires an availability of sets of correct data on the energetic, spectroscopic and structural properties of atoms, especially in the high excited, Rydberg states. Naturally, the correct corresponding data about radiative decay widths, probabilities and oscillator strengths of atomic transitions are needed in building adequate astrophysical models, realizing regular astrophysical, laboratory, thermonuclear plasma diagnostics and in fusion research. Besides, a great interest to studying Rydberg atomic states parameters can be easily explained by a powerful development of such new fields as quantum computing, and quantum cryptography, construction of new type Rydberg atomic lasers etc. Traditionally, considerable attention is devoted to studying the energetic and spectral characteristics of the light atoms (H, He, Li etc) and corresponding multicharged ions. However, studying spectral characteristics of heavy atoms and ions in the Rydberg states has to be more complicated as it requires a necessary accounting the relativistic , exchange-correlations effects and possibly the QED corrections for superheavy atomic systems. There have been sufficiently many reports of calculations and compilation of energies and oscillator strengths for the barium and even Ba-like ions (see, for example, [1–3] and refs. therein), however, an accuracy of theses data call for further serious analysis and calculation. In many papers the Dirac-Fock method, model potential approach, quantum defect approximation in the different realizations have been used for calculating the energy and spectral properties of barium and it has been shown that an account of the polarization interelectron corrections is of a great quantitative importance. The consistent relativistic perturbation theory calculations of the transitions energies and oscillator strengths for some chosen transitions between the Rydberg states are performed in Refs. [4]. However, it should be stated that for majority of the barium Rydberg states and Ba-like ions with high values of a nuclear charge Z, there is not enough precise information available in literatures [1-3]. In our paper the combined relativistic energy approach and relativistic many-body perturbation theory with the zeroth order Dirac-Kohn-Sham 1-particle approximation are used for preliminary estimating the energies and oscillator strengths of radiative transitions from the ground state to the low-excited and Rydberg states, in particular, $6s^2$ -6snp (n =7-50) transitions, of the barium atom. The comparison of the calculated oscillator strengths with available theoretical and experimental (compillated) data is performed. The important point is linked

with non-accounting for the polarization effect contribution into the oscillator strength value that has led to ~30% difference between the empirical (compillated) and theoretical data

2. The theoretical method

In the relativistic energy approach [4-9], which has received a great applications during solving numerous problems of atomic, molecular and nuclear physics (e.g. , see Refs. [10-59]), the imaginary part of electron energy shift of an atom is directly connected with the radiation decay possibility (transition probability). An approach, using the Gell-Mann and Low formula with the QED scattering matrix, is used in treating the relativistic atom. The total energy shift of the state is usually presented in the form:

$$\Delta E = \mathrm{Re}\Delta E + i\,\Gamma/2 \qquad (1)$$

where G is interpreted as the level width, and the decay possibility P = G. The imaginary part of electron energy of the system, which is defined in the lowest order of perturbation theory as [4]:

$$\mathrm{Im}\Delta E(B) = -\frac{e^2}{4\pi} \sum_{\substack{\alpha>n>f \\ [\alpha<n\le f]}} V^{|\omega_{\alpha n}|}_{\alpha n \alpha n} \qquad (2)$$

where (a>n>f) for electron and (a<n<f) for vacancy. The matrix element is determined as follows:

$$V^{|\omega|}_{ijkl} = \iint dr_1 dr_2 \Psi^*_i(r_1)\Psi^*_j(r_2)\frac{\sin|\omega|r_{12}}{r_{12}}(1 - \alpha_1\alpha_2)\Psi^*_k(r_2)\Psi^*_l(r_1) \qquad (3)$$

The separated terms of the sum in (3) represent the contributions of different channels and a probability of the dipole transition is:

$$\Gamma_{\alpha_n} = \frac{1}{4\pi}\cdot V^{|\omega_{\alpha_n}|}_{\alpha_n\alpha_n} \qquad (4)$$

The corresponding oscillator strength:

$$gf = \lambda^2_g \cdot \Gamma_{\alpha_n} / 6.67\cdot 10^{15}$$

where g is the degeneracy degree, l is a wavelength in angstrems (Å). Under calculating the matrix elements (3) one should use the angle symmetry of the task and write the expansion for potential sin|w|r12/r12 on spherical functions as follows [4]:

$$\frac{\sin|\omega|r_{12}}{r_{12}} = \frac{\pi}{2\sqrt{r_1 r_2}}\sum_{\lambda=0}^{\infty}(\lambda)J_{\lambda+1/2}(|\omega|r_1)\cdot J_{\lambda+1/2}(|\omega|r_1)J_{\lambda+1/2}(|\omega|r_2)P_\lambda(\cos \boldsymbol{r}_1\boldsymbol{r}_2) \qquad (5)$$

where J is the Bessel function of first kind and (l)= 2l + 1. This expansion is corresponding to usual multipole one for probability of radiative decay. Substitution of the expansion (5) to matrix element of interaction gives as follows [5-8]:

$$V^{\omega}_{1234} = [(j_1)(j_2)(j_3)(j_4)]^{1/2}\sum_{\lambda\mu}(-1)^{\mu}\begin{pmatrix} j_1 j_3 & \lambda \\ m_1 - m_3 & \mu \end{pmatrix}\times \mathrm{Im}Q_\lambda(1234)$$

$$Q_\lambda = Q^{\mathrm{Cul}}_\lambda + Q^{\mathrm{B}}_\lambda\ , \qquad (6)$$

where j_i is the total single electron momentums, m_i – the projections; Q^{Cul} is the Coulomb part of interaction, Q^{Br} - the Breit part. Their detailed definitions are presented in Refs. [4,20]. The detailed expressions for the Coulomb and Breit parts and the corresponding radial R_l and angular S_l integrals can be found in Refs. [22-32].The total probability of a λ - pole transition is usually represented as a sum of the electric P^E_λ and magnetic P^M_λ parts. The electric (or magnetic) λ - pole transition $\gamma \to \delta$ connects two states with parities which by λ (or λ +1) units. In our designations

$$P^E_\lambda(\gamma\to\delta) = 2(2j+1)Q^E_\lambda(\gamma\delta;\gamma\delta)$$
$$P^M_\lambda(\gamma\to\delta) = 2(2j+1)Q^M_\lambda(\gamma\delta;\gamma\delta) \qquad (7)$$

$$Q^E_\lambda = Q^{Cul}_\lambda + Q^{Br}_{\lambda,\lambda-1} + Q^{Br}_{\lambda,\lambda+1}$$
$$Q^M_\lambda = Q^{Br}_{\lambda,\lambda}. \qquad (8)$$

In our work the relativistic wave functions are determined by solution of the Dirac equation with the potential, which includes the modified Kohn-Sham exchange potential [17] insist of the standard Fock one. The important point of

the many-body calculations is in accurate account of the exchange–correlation effects [5-15]. However, in this preliminary studying the energy and spectroscopic parameters of the barium spectra we are limited by non-accounting for the polarization effect contribution and other correlation corrections. Its consistent and accurate accounting will be considered in the next paper. All calculations are performed on the basis of the modified numeral code Superatom (version 93).

3. Results and conclusion

Table 1, 2 shows the energies and oscillators strengths of the transitions between the terms of the configurations $6s^2$ -6snp (n~50). Taking into account a great size of the obtained data we are limited below only by some data. As it has been underlined above, here during this preliminary studying the energy and spectroscopic parameters of the barium spectra we were limited by non-accounting for the polarization effect contribution and other correlation corrections. By the way, it is well-known that the similar complicated atomic systems, spectra and corresponding computing the radiative parameters require very accurate accounting for the different groups of the many-body exchange-correlation effects (see, for example, refs. [5-25]). Moreover, only such a way is able to provide spectral data with sufficient accuracy for modern spectroscopic applications. Such calculations are now in progress and more full information will be presented in the next papers special Preprint.

Table 1

The energy (cm^{-1}) and the oscillators strengths of $6s^2$ -6snp transitions (see text)

Transition	Terms	E (cm^{-1}) [2]	gf [2]	gf (our)
$6s^2$ -6s13p	^1S-$^1P^o$	40763	2.1-4	1.3-4
$6s^2$ -6s15p	^1S-$^1P^o$	41183	1.4-3	0.8-3
$6s^2$ -6s16p	^1S-$^1P^o$	41306	6.0-4	3.8-4

Table 2

The energy (cm^{-1}) and the oscillators strengths of the $6s^2$ -6snp transitions (n = 16-30; our data)

Transition	Terms	E (cm^{-1})	gf
$6s^2$ -6s16p	^1S-$^1P^o$	41306	3.7-4
$6s^2$ -6s20p	^1S-$^1P^o$	41615	0.6-4
$6s^2$ -6s21p	^1S-$^1P^o$	41662	1.8-5
$6s^2$ -6s30p	^1S-$^1P^o$	41871	2.2-5

We are planning to pay especial attention on the accurate accounting for the different groups of the many-body exchange-correlation effects and consider a problem of using the optimized one-particle representation and account for the polarization effect. It is obvious that a possible estimate of the gauge-non-invariant contributions (the difference between the oscillator strengths values calculated with using the transition operator in the form of length and velocity) will be of order 40%, i.e. results, obtained with using different photon propagator gauges (Coulomb, Landau etc) differ significantly (see [6, 60-62]).

References

1. Luc Koenig E., Aymar M., Van Leeuwen R., Ubachs W., Hogervorst W., The 5d5g states in Ba//Phys.Rev.A-1995.-Vol.52.-P.208-215
2. Klose J., Fuhr J., Wiese W., Critically evaluated atomic transition probabilities for BaI, BaII/ //J. Phys. Ch. Ref. Dat.-2002.-Vol. 31.-P.217-230.
3. Ivanova E.P., Grant I., Oscillator strength anomalies in Ne isoelectronic sequence with applications to X-ray laser modeling// J. Phys. B:At.Mol.Phys.-1998-Vol.31.-P.2871.
4. Ivanov L.N.,Ivanova E.P., Extrapolation of atomic ion energies by model potential method: Na-like spectra// Atom. Data Nucl Data Tab.-1999.-Vol.24.-P.95-121.
5. Ivanov L.N., Ivanova E.P., Knight L., Energy Approach to consistent QED theory for calculation of electron-col-

lision strengths/ //Phys.Rev.A.-1993.-Vol.48.-P.4365-4374.
6. Glushkov A.V.,Ivanov L.N., Radiation Decay of Atomic States: atomic residue polarization and gauge non-invariant contributions//Phys. Lett.A.-1997-Vol.170(1).-P.33-36.
7. Glushkov A.V.,Ivanov L.N., DC Strong-Field Stark-Effect: consistent quantum-mechanical approach//J. Phys.B: At. Mol. Opt. Phys.-1993.-Vol.26.-P.L379-386.
8. Glushkov A.V., Relativistic Quantum Theory. Quantum, mechanics of Atomic Systems.-Odessa: Astroprint, 2008.-700P.
9. 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.-525-541.
10. 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.
11. Glushkov A.V., Khetselius O., Svinarenko A, Relativistic theory of cooperative muon-g 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.
12. 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.
13. 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.
14. Malinovskaya S.V., Glushkov A.V., Khetselius O.Yu., Lopatkin Yu., Loboda A.V., Svinarenko 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,N2.-P.288-296.
15. Malinovskaya S., Glushkov A.V., Khetselius O.Yu., Svinarenko A.A., Mischenko E., Florko T., Optimized perturbation theory scheme for calculating the interatomic potentials and hyperfine lines shift for heavy atoms in the buffer inert gas//Int. J. Quant.Chem.-2009.-Vol.109.-P. 3325-3329.
16. Glushkov A., Malinovskaya S., Prepelitsa G., Ignatenko V., 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.
17. Glushkov A.V., Khetselius O.Yu., Lovett L., Electron-b-Nuclear Spectroscopy of Atoms and Molecules and Chemical Bond Effect on the b-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.
18. 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.
19. Glushkov A., Malinovskaya S., Loboda A., Shpinareva I.,Gurnitskaya E., Korchevsky D., Diagnostics of the colli-

sionally 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.
20. Glushkov A.V., Khetselius O.Yu., Loboda A., Ignatenko A., Svinarenko A., Korchevsky D., Lovett L., QED approach to modeling spectra of the multicharged ions in a plasma: Oscillator and electronion collision strengths//Spectral Line Shapes. AIP Conf.Proc.-2008.-Vol.1058.-P.175-177
21. Malinovskaya S.V., Dubrovskaya Yu.V., Vitavetskaya L.A., Advanced quantum mechanical calculation of the beta decay probabilities// Low Energy Antiproton Phys. AIP Conference Proceedings.-2005.-Vol. 796.-P.201-205.
22. 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.
23. Glushkov A.V., Ambrosov S., Ignatenko A., Korchevsky D., DC Strong Field Stark effect for non-hydrogenic atoms: Consistent quantum mechanical approach// Int.Journ. Quant. Chem.-2004.-Vol.99,N6.-P.936-939.
24. 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. J. Quant. Chem.-2004.-Vol.99.-P.889-893.
25. 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.
26. Malinovskaya S., Glushkov A., Dubrovskaya Yu., Vitavetskaya L., Quantum calculation of cooperative muon-nuclear processes: discharge of metastable nuclei during negative muon capture// Recent Advances in Theory of Chemical and Physical Systems (Springer).-2006.-Vol.15.-P.301-307.
27. Glushkov A.V., Khetselius O.Yu., Loboda A., Svinarenko A., QED approach to atoms in a laser field: Multi-photon resonances and above threshold ionization// Frontiers in Quantum Systems in Chemistry and Physics, Ser.: Progress in Theor.Chem.and Phys.; Eds. S.Wilson, P.Grout, J. Maruani et al, (Springer), 2008.-Vol.18.-P.543-560.
28. Glushkov A.V., Dan'kov S., Prepelitsa G., Polischuk V., Efimov A., Qed theory of nonlinear interaction of the complex atomic systems with laser field multiphoton resonances// Journal of Tech. Phys.-1997.-Vol.38.-P.219-222
29. Glushkov A.V., Ambrosov S.V., Loboda A.V., Gurnitskaya E.P., Khetselius O.Yu., QED calculation of heavy multicharged ions with account for the correlation, radiative and nuclear effects// Recent Advances in Theor. Phys. and Chem. Systems.-2006.-Vol.15.-P.285-299.
30. 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.
31. 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 shileding approximation//Sensor Electr. and Microsyst. Techn.-2007.-N2.-P.9-13
32. 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
33. 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.
34. Glushkov A., Khetselius O., Bunuakova Y., Buyadzhi V., Brusentseva S., Zaichko P., Sensing interaction dynamics of chaotic systems within chaos theory and micro-system technology Geomath with application to neurophysiological systems// Sensor Electr. Microsyst.Techn.-2014-Vol. 11.-P.62
35. 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.
36. Glushkov A.V., Relativistic and correlation effects in spectra of atomic systems.-Odessa: Astroprint.-2006.-400P.
37. Glushkov A.V., Atom in electromagnetic field.-Kiev: KNT, 2005.-450P.
38. Khetselius O.Yu., Hyperfine structure of atomic spectra.-Odessa: Astroprint, 2008.
39. Khetselius O.Yu., Hyperfine structure of radium//Photoelectronics.-2005-N14-P.83-85
40. Khetselius O., Spectroscopy of cooperative electron-gamma-nuclear processes in heavy atoms: NEET effect// J. Phys.: Conf. Ser.-2012.- Vol.397.-P.012012
41. Glushkov A., Malinovskaya S., Gurnitskaya E., Khetselius O.Yu.,Dubrovskaya Yu., 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.
42. 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.
43. Glushkov A., Khetselius O., Svinarenko A., Theoretical spectroscopy of autoionization resonances in spectra of lanthanide atoms// Physica Scripta.-2013.-Vol.T153.-P.014029.
44. Glushkov A., Khetselius O., Gurnitskaya E., Loboda A.,Sukharev D., Relativistic quantum chemistry of heavy ions and hadronic atomic systems: spectra and energy shifts//Theory and Applications of Computational Chemistry. AIP Conf.Proceedings.-2009.-Vol.1102.-P.168-171.
45. Khetselius O.Yu., Relativistic calculating the spectral lines hyperfine structure parameters for heavy ions//Spectral Line Shapes, AIP Conf. Proc.-2008.-Vol.1058.-P.363-365.
46. Khetselius O., Glushkov A., Gurnitskaya E., Loboda A., Mischenko E., Florko T., Sukharev D., Collisional Shift of the Tl hyperfine lines in atmosphere of inert gases// Spectral Line Shapes, AIP Conf. Proc.-2008.-Vol.1058.-P.231-233.
47. Khetselius O.Yu., Hyperfine structure of energy levels for isotopes ^{73}Ge, ^{75}As, ^{201}Hg// Photoelectronics.-2007.-N16.-P.129-132.
48. Khetselius O.Y., Gurnitskaya E.P., Sensing electric and magnetic moments of a nucleus in the N-like ion of Bi// Sensor Electr. and Microsyst. Techn.-2006.-N3.-P.35-39.
49. Khetselius O.Y., Gurnitskaya E.P., Sensing the hyperfine structure and nuclear quadrupole moment for Ra//Sensor Electr. and Microsyst. Techn.-2006.-N2.-P.25-29.
50. 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.
51. 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 atmosphere of inert gas//Phys. Scripta.-2013.-Vol.T153-P. 014037.
52. 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.
53. Khetselius O.,On possibility of sensing nuclei of rare isotopes by means of laser spectroscopy of hyperfine structure// Sensor Electr. Microsyst.Techn.-2008.-Vol.3.-P.28.
54. 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.
55. Buyadzhi V., Chernyakova Yu., Smirnov A., Tkach T., Electron-collisional spectroscopy of atoms and ions in plasma: Be-like ions// Photoelectronics.-2016.-Vol.25.-P.97-101.
56. 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.
57. Glushkov A.V., Khetselius O.Yu., Kuzakon V., Prepelitsa G.P., Solyanikova E.P., Svinarenko A., Modeling of interaction of the non-linear vibrational systems on the basis of temporal series analyses (application to semiconductor quantum generators)// Dynamical Systems- Theory and Applications.-2011.-BIF110.
58. Glushkov A., Khetselius O.Y., Brusentseva S., Zaichko P., Ternovsky V., Studying interaction dynamics of chaotic systems within a non-linear prediction method: application to neurophysiology// Advances in Neural Networks, Fuzzy Systems and Artificial Intelligence, Ser: Recent Adv. in Computer Engineering, Ed. J.Balicki.-2014.-Vol.21.-P.69-75.
59. 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.
60. Glushkov A., Khetselius O., Prepelitsa G., Svinarenko A., Geometry of Chaos: Theoretical basis's of a consistent combined approach to treating chaotic dynamical systems and their parameters determination //Proc. Int. Geometry Center".-2013.-Vol.6, N1.-P.43-48.
61. Svinarenko A., Nikola L., Prepelitsa G., Tkach T., Mischenko E., Auger (autoioni-zation) decay of excited states in spectra of multicharged ions: Relativistic theory//AIP Conf. Proc.-2010.-Vol.1290, N1 P.94-98.
62. Florko T.A., Ignatenko A.V., Svinarenko A.A., Tkach T.B., Ternovsky V.B, Advanced relativistic model potential approach to calculation of the radiation transition and ionization characteristics for Rydberg atoms// Photoelectronics.-2014.-Vol.23.-P.91-95.

This article has been received in May 2017

UDC 539.182

E. V. Ternovsky, O. A. Antoshkina, T. A. Florko, T. B. Tkach

RELATIVISTIC CALCULATION OF OSCILLATOR STRENGTHS OF THE RADIATION TRANSITIONS BETWEEN BARIUM RYDBERG STATES

Summary

The combined relativistic energy approach and relativistic many-body perturbation theory with the zeroth order Dirac-Kohn-Sham one-particle approximation are used for preliminary estimating the energies and oscillator strengths of radiative transitions from the ground state to the low-excited and Rydberg states, in particular, $6s^2$ -6snp (n =7-50) transitions, of the barium atom. The comparison of the calculated oscillator strengths with available theoretical and experimental (compillated) data is performed. The important point is linked with non-accounting for the polarization effect contribution into the oscillator strength value that has led to ~40% difference between the empirical (compillated) and theoretical data.

Key words: relativistic theory, oscillator strengths, radiative transitions

УДК 539.182

Е. В. Терновский, О. А. Антошкина, Т. А. Флорко, Т. Б. Ткач

РЕЛЯТИВИСТСКИЙ РАСЧЕТ СИЛ ОСЦИЛЛЯТОРОВ РАДИАЦИОННЫХ ПЕРЕХОДОВ МЕЖДУ РИДБЕРГОВСКИМИ СОСТОЯНИЯМИ БАРИЯ

Резюме

Комбинированный релятивистский энергитический подход и релятивистская теория возмущений многих тел с дирак-кон-шэмовским одночастичным приближением нулевого порядка используются для предварительной оценки энергий и сил осцилляторов радиационных переходов из основного состояния в низкие возбужденные и ридберговские состояния, в частности, $6s^2$ -6snp (n =7-50) переходоваирма бария. Выполнено сравнение расчетных сил осцилляторов с имеющимися теоретическими и экспериментальными данными. Важнейшая особенность связана с неучетом вклада в величину силы осцилятора, обусловленного эффектом поляризации остова и некоторіми другими корреляционными поправками, что приводит к ~40% отличию между экспериментальными (компиллированными) и теоретическими данными.

Ключевые слова: релятивистская теория, силы осцилляторов, радиационные переходы.

УДК 539.182

Є. В. Терновський, О. О. Антошкіна, Т. О. Флорко, Т. Б. Ткач

РЕЛЯТИВІСТСЬКИЙ РОЗРАХУНОК СИЛ ОСЦИЛЯТОРІВ РАДІАЦІЙНИХ ПЕРЕХОДІВ МІЖ РІДБЕРГІВСЬКИМИ СТАНАМИ БАРІЯ

Резюме

Комбінований релятивістський енергетичний підхід і релятивістська багаточастинкова теорія збурень з дірак-кон-шемівським одночастинковим наближенням нульового порядку використовуються для попередньої оцінки енергій і сил осциляторів радіаційних переходів з основного стану в низько збуджені і рідбергівські стани, зокрема, 6s2 -6snp (n = 7 -50) переходів атома барія. Виконано порівняння розрахункових сил осциляторів з наявними теоретичними і експериментальними даними. Найважливіша особливість даного розрахунку пов'язана з неврахуванням вкладу в величину сили осцилятора, обумовленого ефектом поляризації остова та декотрими іншими кореляційними поправками, що призводить до ~ 40% відмінності між експериментальними (компіллірованними) і теоретичними даними.

Ключові слова: релятивістська теорія, сили осцилляторів, радіаційнні переходи, рідбергівські стани.

UDC 539.185

M. Yu. Gurskaya, A. V. Ignatenko, A. S. Kvasikova, A. A. Buyadzhi

Odessa State Environmental University, 15, Lvovskaya str., Odessa, 65016
e-mail: ignatenkoav13@gmail.com

ADVANCED DATA FOR HYDROGEN ATOM IN CROSSED ELECTRIC AND MAGNETIC FIELDS

Spectroscopy of atoms in the crossed external electric and magnetic fields is investigated on the basis of the operator perturbation theory. As a novel element within the operator perturbation theory, we use more flexible functions for model function, which imitates an electric field. In a case of the crossed electric and magnetic fields we develop more effective finite differences numerical scheme. As illustration, some advanced data for the hydrogen atom in the electric and crossed external electric and magnetic fields are listed. Advanced data for hydrogen atom are listed.

1. Introduction

From the standard quantum mechanics it is well known that the external electric field shifts and broadens the bound state atomic levels. One should note that the usual quantum-mechanical approach relates complex eigen-energies (EE) $E=E_r+0{,}5iG$ and complex eigen-functions (EF) to the shape resonances [1-6]. The calculation difficulties in the standard quantum mechanical approach are well known and described in many Refs. Let us remind that the usual quasiclassical WKB approximation overcomes these difficulties for the states, lying far from "new continuum " boundary and, as rule, is applied in the case of a relatively weak electric field. The same is regarding the widespread asymptotic phase method (c.f.[2]). Quite another calculation procedures are used in the Borel summation of the divergent perturbation theory (PT) series and in the numerical solution of the difference equations following from expansion of the wave function over finite basis [2,3,9,10].

Experimental observation of the Stark effect in a constant (DC) electric field near threshold in hydrogen and alkali atoms led to the discovery of resonances extending into the ionization continuum (c.f.[1]). Calculation of the characteristics of these resonances as well as the Stark resonances in the strong electric field and crossed electric and magnetic fields remains very important problem of as modern atomic physics [1-20].

In this paper we go on our studying of sspectroscopy of atoms in the crossed external electric and magnetic fields. Our method of studying is based on the known formalism of the operator perturbation theory (OPT) [1-3]. According to [1-5], the essence of operator perturbation theory approach is the inclusion of the well known method of "distorted waves approximation" in the frame of the formally exact perturbation theory. As a novel element within the operator perturbation theory, we use more flexible functions for model function, which imitates an electric field. In a case of the crossed electric and magnetic fields we develop more effective finite differences numerical scheme. As illustration, some advanced data for the hydrogen atom in the electric and crossed external electric and magnetic fields are listed.

2. Method of operator perturbation theory

As our approach to strong field DC Stark effect was presented in a series of papers (see, for example, [1-6]), here we are limited only by the key aspects. According to [2,3], the Schrödinger equation for the electronic eigen-function taking into account the uniform DC electric field (the field strength is F)and the field of the nucleus (Coulomb units are used: a unit is $h^2/Ze^2\,m$ and a

unit of mZ^2e^4/h^2 for energy) looks like:

$$[-(1 - N/Z) / r + F z - 0{,}5\Delta - E]\ \psi = 0 \qquad (1)$$

where E is the electronic energy, Z — charge of nucleus, N — the number of electrons in atomic core. Our approach allow to use more adequate forms for the core potential (c.f.[25-27]). According to standard quantum defect theory (c.f.[3]), relation between quantum defect value μ_l, electron energy E and principal quantum number n is: $\mu_l = n - z^*(-2E)^{-1/2}$. As it is known, in an electric field all the electron states can be classified due to quantum numbers: n, n_1, n_2, m (principal, parabolic, azimuthal: $n = n_1 + n_2 + m + 1$). Then the quantum defect in the parabolic co-ordinates $\delta(n_1 n_2 m)$ is connected with the quantum defect value of the free ($F=0$) atom by the following relation [3]:

$$\delta(n_1 n_2 m) = (1/n) \sum_{l=m}^{n-1} (2l+1)(C^{JM}_{J,M-m;lm})^2 \mu_l$$
$$J=(n-1)/2,\ \ M=(n_1-n_2+m)/2;$$

After separation of variables, equation (1) in parabolic co-ordinates could be transformed to the system of two equations for the functions f and g:

$$f'' + \frac{|m|+1}{t} f' + [0{,}5E + (\beta_1 - N/Z) / t - 0{,}25\ F(t)\ t\ ] f = 0 \qquad (2)$$

$$g'' + \frac{|m|+1}{t} g' + [0{,}5E + \beta_2 / t + 0{,}25\ F(t)\ t\ ] g = 0 \qquad (3)$$

coupled through the constraint on the separation constants: $\beta_1 + \beta_2 = 1$.

For the uniform electric field $F(t) = F$. In ref. [11], the uniform electric field ε in (3) and (4) was substituted by model function F(t) with parameter τ ($\tau = 1.5\, t_2$). To simplify the calculation procedure, the uniform electric field ε in (3) and (4) should be substituted by the function [57,58]:

$$\varepsilon(t) = \frac{1}{t}\ \varepsilon\left[(t-\tau)\frac{\tau^4}{\tau^4 + t^4} + \tau\right] \qquad (4)$$

th sufficiently large τ ($\tau = 1.5 t_2$). The function $\varepsilon(t)$ practically coincides with the constant ε in the inner barrier motion region ($t < t_2$) and disappears at $t >> t_2$. Potential energy in equation (4) has the barrier. Two turning points for the classical motion along the η axis, t_1 and t_2, at a given energy E are the solutions of the quadratic equation ($\beta = \beta_1$, $E = E_0$). According to [1-3], one should know two zeroth order EF of the H_0: bound state function Ψ_{Eb} (ε, ν, φ) and scattering state function Ψ_{Es} (ε, η, φ) with the same EE in order to calculate the width G of the concrete quasi-stationary state in the lowest PT order. Firstly, one would have to define the EE of the expected bound state. It is the well known problem of states quantification in the case of the penetrable barrier. Further one should solve the system (2, 3) system with the total Hamiltonian H using the conditions [11]:

$$f(t) \to 0 \text{ at } t \Rightarrow \infty$$
with
$$\partial x(\beta, E) / \partial E = 0 \qquad (5)$$
$$x(\beta, E) = \lim_{t \Rightarrow \infty} [\ g^2(t) + \{g'(t) / k\}^2\ ]\ t^{|m|+1}.$$

These two conditions quantify the bounding energy E, with separation constant β_1. The further procedure for this two-dimensional eigenvalue problem results in solving of the system of the ordinary differential equations(2, 3) with probe pairs of E, β_1. The bound state EE, eigenvalue β_1 and EF for the zero order Hamiltonian H_0 coincide with those for the total Hamiltonian H at $\varepsilon \Rightarrow 0$, where all the states can be classified due to quantum numbers: n, n_1, l, m (principal, parabolic, azimuthal) that are connected with E, β_1, m by the well known expressions.. The scattering states' functions must be orthogonal to the above defined bound state functions and to each other. According to the OPT ideology [11,12], the following form of $g_{E's}$:is possible:

$$g_{E's}(t) = g_1(t) - z_2'\, g_2(t) \qquad (6)$$

with $f_{E's}$, and $g_1(t)$ satisfying the differential equations (2) and (3). The function g_2(t) satisfies the non-homogeneous differential equation, which differs from (3) only by the right hand term, disappearing at $t \Rightarrow \infty$.

In Ref, [7] it has been presented approach, based on solution of the 2-dimensional Schrödinger equation for an atomic system in crossed fields and operator perturbation theory. For definiteness, we consider a dynamics of the complex non-coulomb atomic systems in a static magnetic and electric fields. The hamiltonian of the multi-electron atom in a static magnetic and electric fields is (in atomic units) as follows:

$$H = 1/2(p_\rho^2 + l_z^2/\rho^2) + B_z/2 + (1/8)B^2\rho^2 + \\ + (1/2)p_z^2 + F + V(r) \quad (7)$$

where the electric field F and magnetic field B are taken along the z-axis in a cylindrical system; In atomic units: 1 a.u.B=2.35×10^{5}T, 1a.u.F=5,144×10^6 kV/cm. For solution of the Schrödinger equation with hamiltonian equations (7) we constructed the finite differences scheme which is in some aspects similar to method [7]. An infinite region is exchanged by a rectangular region: $0<\rho< L_\rho$, $0<z< L_Z$. It has sufficiently large size; inside it a rectangular uniform grid with steps h_ρ, h_Z was constructed. The external boundary condition, as usually, is: $(\partial\Psi/\partial n)_\Gamma = 0$.

The knowledge of the asymptotic behaviour of wave function in the infinity allows to get numeral estimates for L_ρ, L_Z. A wave function has an asymptotic of the kind as: *exp[-(-2E)$^{1/2}$r*], where *(-E)* is the ionization energy from stationary state to lowest Landau level. Then L can be estimated as $L\sim 9(-2E)^{-1/2}$. The more exact estimate is found empirically. The finite-difference scheme is constructed as follows. The three-point symmetric differences scheme is used for second derivative on z. The derivatives on ρ are approximated by (2m+1)-point symmetric differences scheme with the use of the Lagrange interpolation formula differentiation. To calculate the values of the width G for resonances in atomic spectra in an electric field and crossed electric and magnetic field one can use the modified operator perturbation theory method (see details in ref.[10,20]). Note that the imaginary part of the state energy in the lowest PT order is:

$$\mathrm{Im}\,E = G/2 = \pi < \Psi_{Eb} \mid H \mid \Psi_{Es} >^2 \quad (8)$$

with the total Hamiltonian of system in an electric and magnetic field. The state functions Ψ_{Eb} and Ψ_{Es} are assumed to be normalized to unity and by the δ(k -k')-condition, accordingly. Other calculation details can be found in ref. [7]. Different application are considered in Refs. [21-57].

3. Illustration results and conclusion

As an illustration,, we make computing the energy of the ground state of the hydrogen atom in crossed fields and compare results with data obtained within analytical perturbation theory by TurbinerV (see. [8]) for the case of sufficiently weak fields. Table 1 shows the values of the energy of the ground state of the hydrogen atom (the following designations: $E+E^{||}$ - energy for the case of the electric and magnetic fields are parallel; $E+E^{\perp}$ corresponds to the case of the electric and magnetic fields are perpendicular).

Table 1

Energy values (Ry) of the H ground state in electric F (1au=5.14·10^9 V/cm) and magnetic B (1 au.B=2.35·10^5 T) fields

F,B 10^{-2}	$E+E^{\|\|}$ Turbiner theory [8]	$E+E^{\|\|}$ [5]
0,0	-1,000000	-1,000000
0,1	-1,000004	-1,000004
0,5	-1,000099	-1,000099
1,0	-1,000402	-1,000401
1,5	-1,000906	-1,000905
2,0	-1,001617	-1,001616
2,5	-1,002542	-1,002540
3,0	-1,003685	-1,003682
3,5	-1,005054	-1,005053
4,0	-1,0066619	-1,006659
4,5	-1,008520	-1,008517
5,0	-1,010642	-1,010636
F,B 10-2	$E+E^{\|\|}$ This work	$E+E^{\perp}$ This work
0,0	-1,000000	-1,000000
0,1	-1,000004	-1,000004
0,5	-1,000100	-1,000099
1,0	-1,000402	-1,000401
1,5	-1,000906	-1,000905
2,0	-1,001617	-1,001616
2,5	-1,002541	-1,002535
3,0	-1,003684	-1,003673
3,5	-1,005054	-1,005036
4,0	-1,006686	-1,006627
4,5	-1,008519	-1,008464
5,0	-1,010638	-1,010556

Since the considered electric field is sufficiently weak, difference between all data in Table 1 is quite little. At the same time it is clear that the perturbation theory in the standard quantum-mechanical version is correct exclusively for the weak fields, while for strong fields it can lead to substantially inaccurate data. Really, in Table 2 we list the results for the Stark resonances energies and widths of the ground state hydrogen atom in the DC electric field with the strength ε=0.1 and 0.8 a.u., obtained within the most exact alternative methods and our data (see [2]).

Table 2

The energies and widths of the Stark resonances of the H ground state (F=0.1, 0.8 a.u.). Notation: (A) Hehenberger, H.V. McIntosh and E. Brändas, (B) Farrelly and Reinhardt, (C) Rao, Liu and Li [18], (D) Glushkov-Ivanov, the standard OPT method; (E)- Popov et al; (F) – our data

F, a.u.	Method	Er, a.u.	Γ/2, a.u.
0.10	A	-0.52743	0.725×10^{-2}
	C	-0.527418	0.7269×10^{-2}
	D	-0.527419	0.2269×10^{-2}
	E	-0.527	0.227×10^{-2}
	F	-0.527418	0.7269×10^{-2}
0.80	B	-0.6304	0.5023
	C	-0.630415	0.50232
	D	-0.630416	0.50232
	F	-0.630415	0.50231

The comparison of our data (Table 2: F) with earlier similar results, obtained within the summation of divergent PT series, the numerical solution with expansion of the wave function over finite basis, a complex scaling plus B-spline calculation, the standard OPT one (Table 2: A-E) shows quite acceptable agreement. We believe that the OPT method with new elements will be especially efficient for atoms in the strong crossed electric and magnetic fields, where the standard methods (usual perturbation theory etc) deal with great principal and computational problems).

References

1. Glushkov A.V., Atom in electromagnetic field.-Kiev: KNT, 2005.-400P.
2. 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.
3. Glushkov A.V.,Ivanov L.N. DC Strong-Field Stark-Effect: Consistent Quantum-mechanical Approach // J. Phys. B: At. Mol. Opt. Phys.-1993.-Vol.26,N16.- P.L379-L386.
4. 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,N5.-P.936-939.
5. 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.
6. Fedchuk A.P., Glushkov A.V., Lepikh Ya.I., Ignatenko A.V., Kvasikova A.S., Atom of hydrogen and wannier-mott exciton in crossed electric and magnetic fieldst// Photoelectronics.-2014.-Vol.23.-P.176-181.
7. Kvasikova A.S., Ignatenko A.V., Florko T.A., Sukharev D.E., Chernyakova Yu.G., Photoeffect and spectroscopy of the hydrogen atom in the crossed dc electric and magnetic field//Photoelectronics.-2011.-Vol.20.-P.71-75.
8. Lisitsa V.S. New in Stark and Zeemane effects for Hydrogen Atom// Phys. Uspekhi.- 1987.-Vol.153.- P.379-422.
9. Popov V.S., Mur V.D., Sergeev A.V., Weinberg V.M., Strong field Stark effect: perturbation theory and 1/n expansion//Phys. Lett. A.-1990.-V.149.-P.418-424
10. 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.
11. Glushkov A.V., Malinovskaya S.V., Ambrosov S., Shpinareva I.M., Troitskaya O., Resonances in quantum systems in strong external fields consistent quantum approach// J. Techn.Phys.-1997.-Vol.38, N2.-P.215-218.
12. 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.
13. 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
14. 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.
15. Glushkov A.V., Energy approach to resonance states of compound super-heavy nuclei and EPPP in heavy nucleus collisions// Low Energy Antiproton Phys. AIP Conference Proceedings.-2005.-Vol.796.-P.206-210.
16. 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.
17. 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.
18. 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.
19. 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. J. Quant. Chem.-2004.-Vol.99.-P.889-893.
20. 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.
21. 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
22. Glushkov A.V., Ambrosov S.V., Loboda A.V., Gurnitskaya E.P., Khetselius O.Yu., QED calculation of heavy multicharged ions with account for the correlation, radiative and nuclear effects// Recent Advances in Theor. Phys. and Chem. Systems.-2006.-Vol.15.-P.285.
23. 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.
24. 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 shileding approximation// Sensor Electr. and Microsyst. Techn.-2007.-N2.-P.9-13
25. 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.
26. 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.
27. 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.
28. Prepelitsa G.P., Glushkov A.V., Lepikh Ya.I., Buyadzhi V.V., Ternovsky V.B., Zaichko P.A., Chaotic dynamics of non-linear 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.
29. Glushkov A.V., Relativistic and correlation effects in spectra of atomic systems.-Odessa: Astroprint.-2006.-400P.
30. Khetselius O.Yu., Hyperfine structure of atomic spectra.-Odessa: Astroprint, 2008.-210P.
31. Khetselius O.Yu., Hyperfine structure of radium// Photoelectronics.-2005.-N14.-P.83-85.
32. Khetselius O., Spectroscopy of cooperative electron-gamma-nuclear processes in heavy atoms: NEET effect// J. Phys.: Conf. Ser.-2012.- Vol.397.-P.012012
33. 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.
34. 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.
35. 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.
36. Glushkov A., Malinovskaya S., Gurnitskaya E., Khetselius O.Yu.,Dubrovskaya Yu., 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.
37. Glushkov A.V., Khetselius O.Y., Brusentseva S.V., Zaichko P.A., Ternovsky V.B., Studying interaction dynamics of chaotic systems within a non-linear prediction method: application to neurophysiology// Advances in Neural Networks, Fuzzy Systems and Artificial Intelligence, Ser: Recent Adv. in Computer Engineering, Ed. J.Balicki.-2014.-Vol.21.-P.69-75.
38. Khetselius O.Yu., Quantum Geometry: New approach to quantization of the quasistationary states of Dirac equation for super heavy ion and calculating hyper fine structure parameters// Proc. Int.Geometry Center.-2012.-Vol.5,№ 3-4.-P.39-45.
39. 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.
40. 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.
41. 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.
42. 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. Proc.-2008.-Vol.1058.-P.231-233.
43. Khetselius O.Yu., Hyperfine structure of energy levels for isotopes 73Ge, 75As, 201Hg// Photoelectronics.-2007.-N16.-P.129-132.
44. 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.
45. 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.
46. 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.
47. 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.
48. Glushkov A.V., Khetselius O.Yu., Kuzakon V., Prepelitsa G.P., Solyanikova E.P., Svinarenko A., Modeling of interaction of the non-linear vibrational systems on the basis of temporal series analyses (application to semiconductor quantum generators)// Dynamical Systems-Theory and Applications.-2011.-BIF110.
49. Svinarenko A.A., Nikola L. V., Prepelitsa G., Tkach T.B, Mischenko E.V., Auger (autoionization) decay of excited states in spectra of multicharged ions: Relativistic theory//AIP Conf. Proc.-2010.-Vol.1290, N1 P.94-98.
50. 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.-525-541.
51. 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.
52. Glushkov A.V., Khetselius O., Svinarenko 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.
53. 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.
54. 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.
55. Glushkov A.V., Khetselius O.Yu., Prepelitsa G., 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 International Geometry Center».-2013.-Vol.6, N1.-P.43-48.
56. 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.
57. Glushkov A.V., Khetselius O.Yu., Loboda A.V., Svinarenko A.A., QED approach to atoms in a laser field: Multi-photon 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.

This article has been received in May 2017

UDC 539.185

M. Yu. Gurskaya, A. V. Ignatenko, A. S. Kvasikova, A. A. Buyadzhi

ADVANCED DATA FOR HYDROGEN ATOM IN CROSSED ELECTRIC AND MAGNETIC FIELDS

Summary

Spectroscopy of atoms in the crossed external electric and magnetic fields is investigated on the basis of the operator perturbation theory. As a novel element within the operator perturbation theory, we use more flexible functions for model function, which imitates an electric field. In a case of the crossed electric and magnetic fields we develop more effective finite differences numerical scheme. As illustration, some advanced data for the hydrogen atom in the electric and crossed external electric and magnetic fields are listed. Advanced data for hydrogen atom are listed.

Key words: atom, hydrogen, crossed electric and magnetic fields

УДК 539.185

М. Ю. Гурская, А. В. Ігнатенко, А. С. Квасикова, А. А. Буяджи

АТОМ ВОДОРОДА В СКРЕЩЕННЫХ ЭЛЕКТРИЧЕСКОМ И МАГНИТНОМ ПОЛЯХ

Резюме

Работа посвящена изучению спектроскопических параметров атомов в постоянном электрическом и скрещенных электрическом и магнитном полях на основе формализма известной операторной теории возмущений. В качестве нового элемента в операторную теорию возмущений оператора вводится применение более эффективной функции для модельной функции, имитирующей электрическое поле. В случае скрещенных электрического и магнитного полей разработана более эффективная численная конечно-разностная схема. В качестве иллюстрации приведены некоторые уточненные данные для атома водорода в сильном электрическом поле и скрещенных электрическом и магнитном полях. Приведены численные данные для атома водорода.

Ключевые слова: атом, водород, скрещенные электрическое и магнитное поля

УДК 539.185

М. Ю. Гурська, Г. В. Ігнатенко, Г. С. Квасікова, Г. А. Буяджі

АТОМ ВОДНЮ В СХРЕЩЕНИХ ЕЛЕКТРИЧНОМУ І МАГНІТНОМУ ПОЛЯХ

Резюме

Робота присвячена вивченню спектроскопічних параметрів атомів у сталому електричному та схрещених електричному та магнітному полях на основі відомої операторної теорії збурень. В якості нового елементу в операторну теорію збурень вводиться використання більш ефективної функції для модельної функції, яка імітує зовнішнє електричне поле. У випадку схрещених електричного та магнітного полей розроблена ефективна чисельна скінченно-різницева схема. В якості ілюстрації наведені уточнені данні для атома водню в сильному електричному полі і схрещених електричному та магнітному полях полях. Наведено чисельні дані для атома водню.

Ключові слова: атом, водень, схрещені електричне і магнітне поля

PACS: 73.20.Hb, 73.25.+I; UDC 621.315.592

O. O. Ptashchenko[1], F. O. Ptashchenko[2], V, R.Gilmutdinova[1]

EFFECT OF WATER VAPORS ON THE TIME-RESOLVED SURFACE CURRENT INDUCED BY AMMONIA MOLECULES ADSORPTION IN GaAs *P-N* JUNCTIONS

[1]I. I. Mechnikov National University of Odessa, Dvoryanska St., 2, Odessa, 65026, Ukraine
[2]National University "Odessa Maritime Academy", Odessa, Didrikhsona St., 8, Odessa, 65029, Ukraine

Supplement to the article published in Photoelectronics. – 2016. – № 25. – P. 126–131.

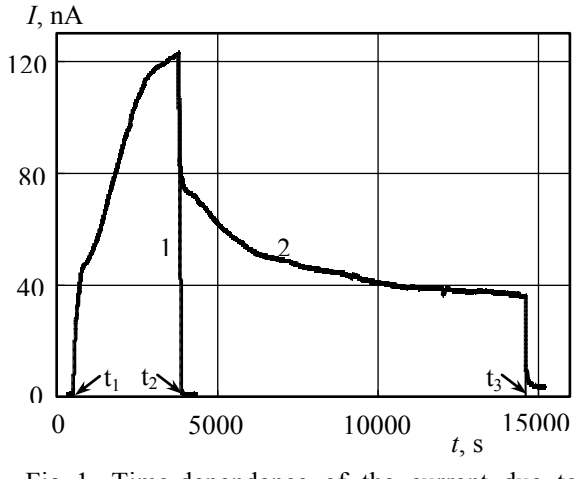


Fig. 1. Time-dependence of the current due to atmosphere changing: 1– dry air → (t_1) NH_3+H_2O vapors → (t_2) dry air; 2– dry air → (t_1) NH_3+H_2O vapors → (t_2) H_2O vapors→ (t_3) dry air.

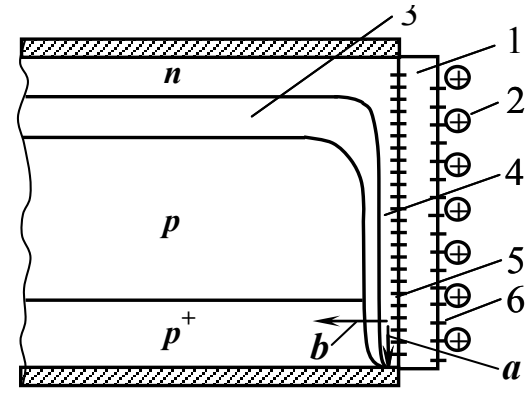


Fig 3. Schematic of a *p-n* structure, placed in a donor gas: 1 – oxide layer; 2 – ions; 3 – depletion layer; 4 – conducting channel; 5 – surface (fast) centers; 6 – states on the oxide surface (slow centers). Arrows: *a* – direction of the electron movement along the channel; b – tunneling from the channel into the p^+ region.

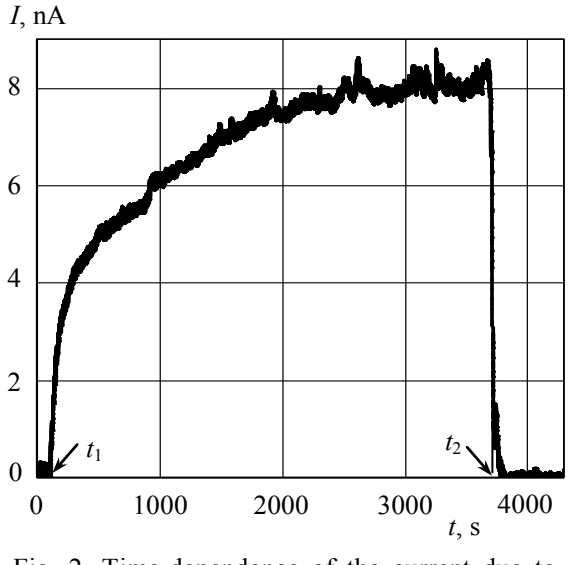


Fig. 2. Time-dependence of the current due to the ambient atmosphere changing: dry air → (t_1) H_2O vapors → (t_2) dry air.

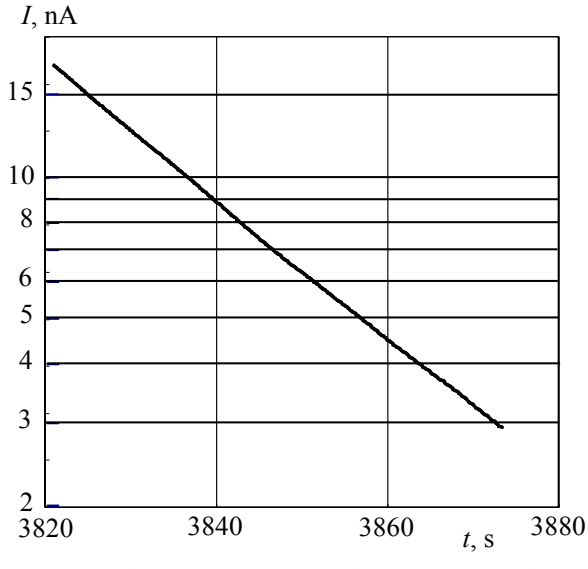


Fig. 4a. The "fast" exponential component of the curve 2 decay section in Fig. 1.

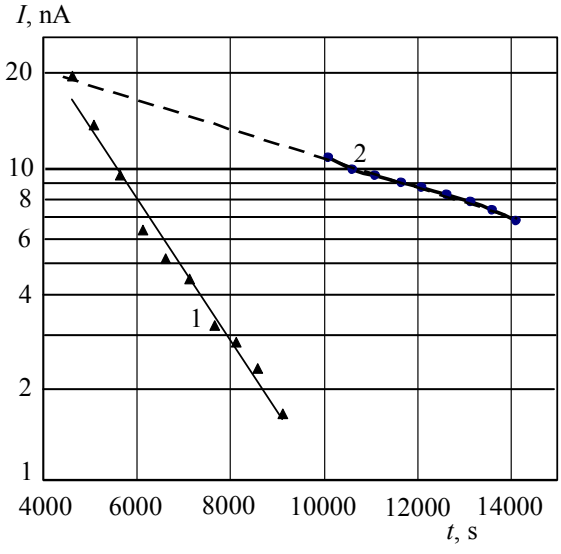


Fig. 4b. Two "slow" exponential components of the curve 2 decay section in Fig. 1.

Інформація для авторів наукового збірника «Photoelectronics»

У збірнику "Photoelectronics " друкуються статті, що містять відомості про наукові дослідження і технічні розробки в напрямках:

*** фізика напівпровідників;**
*** гетеро- і низькорозмірні структури;**
*** фізика мікроелектронних приладів;**
*** лінійна і нелінійна оптика твердого тіла;**
*** оптоелектроніка та оптоелектронні прилади;**
*** квантова електроніка;**
*** сенсорика**

Збірник "Photoelectronics видається англійською мовою. Рукопис подається автором у двох примірниках англійською і російською мовами.

Електронна копія статті повинна відповідати наступним вимогам:
1. Для тексту дозволяються наступні формати - MS Word (rtf, doc).
2. Рисунки приймаються у форматах – EPS. TIFF. BMP, PCX, JPG. GIF, CDR. WMF, MS Word I MS Giaf, Micro Calc Origin (opj).

Рукописи надсилаються за адресою:
Відп. секр. Куталовій М. І., вул. Пастера, 42. фіз. фак. ОНУ, м. Одеса, 65082
E-mail: photoelectronics@onu.du.ua
тел. 0482 0482 723 34 61.

Збірники "Photoelectronics" знаходяться на сайті: http://photoelectronics.onu.edu.ua

До рукопису додаються:
1. Коди PAC і УДК. Допускається використання декількох шифрів, що розділяються комами.
2. Прізвища і ініціали авторів.
3. Установа, повна поштова адреса, номер телефону, номер факсу, адреси електронної пошти для кожного з авторів.
4. Назва статті.
5. Резюме обсягом до 200 слів пишеться англійською, російськоюю і (для авторів з України) – українською мовами.

Текст друкувати шрифтом 14 пунктів через два інтервали на білому папері формату А4. Назва статті, а також заголовки підрозділів друкуються прописними літерами. .

Рівняння необхідно друкувати в редакторі формул MS Equation Editor. Необхідно давати визначення величин, що з'являються в тексті вперше.

Посилання на літературу друкувати через два інтервали, нумеруватися в квадратних дужках послідовно, у порядку їхньої появи в тексті статті. Посилатися необхідно на літературу, що видана пізніше 2000 року.

Підписи до рисунків і таблиць друкуються в тексті рукопису в порядку їхньої ілюстрації.

Резюме обсягом до 200 слів друкується англійською, російською і українською мовами (для авторів з України). Перед текстом резюме відповідною мовою вказуються УДК, прізвища та ініціали всіх авторів, назва статті.

Информация для авторов
Научного сборника «Photoelectronics»

В сборнике "Photoelectronics " печатаются статьи, которые содержат сведения о научных исследованиях и технических разработках в направ-лениях:

*** физика полупроводников;**
*** гетеро- и низкоразмерные структуры;**
*** физика микроэлектронных приборов;**
*** линейная и нелинейная оптика твердого тела;**
*** оптоэлектроника и оптоэлектронные приборы;**
*** квантовая электроника;**
*** сенсорика**

Сборник"Photoelectronics издаётся на английском языке. Рукопись подается автором в двух экземплярах на английском и русском языках.

Электронная копия статьи должна отвечать следующим требованиям:
1. Для текста допустимы следующие форматы - MS Word (rtf, doc).
2. Рисунки принимаются в форматах – EPS. TIFF. BMP, PCX, JPG. GIF, CDR. WMF, MS Word И MS Giaf, Micro Calc Origin (opj).

Рукописи присылаются по адресу:
Отв. секр. Куталовой М. И., ул. Пастера. 42. физ. фак. ОНУ, г. Одесса, 65026
E-mail:photoelectronics@onu.du.ua тел. 0482 723 34 61.

Статьи сб."Photoelectronics " находятся на сайте: http://photoelectronics.onu.edu.ua

К рукописи прилагается:
1. Коды PAC и УДК. Допускается использование нескольких шифров, которые разделяются запятой.
2. Фамилии и инициалы авторов.
3. Учреждение, полный почтовый адрес, номер телефона, номер факса, адреса электронной почты для каждого из авторов.
4. Название статьи.
5. Резюме объемом до 200 слов пишется на английском, русском языках и (для авторов из Украины) – на украинском.

Текст должен печататься шрифтом 14 пунктов через два интервала на белой бумаге формата А4. Название статьи, а также заголовки подразделов печатаются прописными буквами и отмечаются полужирным шрифтом.

Уравнения необходимо печатать в редакторе формул MS Equation Editor. Необходимо давать определение величин, которые появляются в тексте впервые.

Ссылки на литературу должны печататься через два интервала, нумероваться в квадратных скобках последовательно, в порядке их появления в тексте статьи. Ссылаться необходимо на литературу, которая издана позднее 2000 года.

Подписи к рисункам и таблицам печатаются в тексте рукописи в порядке их иллюстрации.

Резюме объемом до 200 слов печатается на английском, русском языках и на украинском (для авторов из Украины). Перед текстом резюме соответствующим языком указываются УДК, фамилии и инициалы всех авторов, название статьи.

Information for contributors of «Photoelectronics» articles

"Photoelectronics" Articles publishes the papers which contain information about scientific research and technical designs in the following areas:

- Physics of semiconductors;
- Physics of microelectronic devices;
- Linear and non-linear optics of solids;
- Optoelectronics and optoelectronic devices;
- Quantum electronics;
- Sensorics.

"Photoelectronics" Articles is defined by the decision of the Highest Certifying Commission as the specialized edition for physical-mathematical and technical sciences and published and printed at the expense of budget items of Odessa I. I. Mechnikov National University.

«Photoelectronics» Articles is published in English. Authors send two copies of papers in English. The texts are accompanied by 3.5» diskette with text file, tables and figures. Electronic copy of a material can be sent by e-mail to the Editorial Board and should meet the following requirements:

1.The following formats are applicable for texts – MS Word (rtf, doc).

2. Figures should be made in formats – EPS, TIFF, BMP, PCX, JPG, GIF, WMF, MS Word I MS Giaf, Micro Calc Origin (opj). Figures made by packets of mathematical and statistic processing should be converted into the foregoing graphic formats.

The papers should be sent to the address:

Kutalova M.I., Physical Faculty of Odessa I.I. Mechnikov National University, 42 Pastera str, 65026 Odessa, Ukraine, e-mail: wadz@mail.ru, tel. +38-0482 723 34 61. Information is on the site:

http://www.photoelectronics.onu.edu.ua

The title page should contain:

1. Codes of PACS
2. Surnames and initials of authors
3. TITLE OF PAPER
4. Name of institution, full postal address, number of telephone and fax, electronic address

An abstract of paper should be not more than 200 words. Before a text of summary a title of paper, surnames and initials of authors should be placed.

Equations are printed in MS Equation Editor.

References should be printed in double space and should be numbered in square brackets consecutively throughout the text. References for literature published in 2000-2009 years are preferential.

Illustrations will be scanned for digital reproduction. Only high-quality illustrations will be taken for publication. Legends and symbols should be printed inside. Neither negatives, nor slides will be taken for publication. All figures (illustrations) should be numbered in the sequence of their record in text.

For additional information please contact with the Editorial Board.

Комп'ютерне верстання – О. І. Карлічук

Підп.до друку 27.11.2017. Формат 60×84/8.
Ум.-друк. арк. 18,83. Тираж 300 пр. Зам. № 1606.

Видавець і виготовлювач
Одеський національний університет імені І. І. Мечникова

Свідоцтво суб'єкта видавничої справи ДК № 4215 від 22.11.2011 р.

Україна, 65082, м. Одеса, вул. Єлісаветинська, 12
Тел.: (048) 723 28 39