PACS 32.30.-r

A. V. Glushkov, I. S. Cherkasova, V. B. Ternovsky, A. A. Svinarenko

Odessa State Environmental University, L'vovskaya str.15, Odessa, 65016
E-mail: svinarenkoaa@gmail.com

THEORETICAL STUDYING SPECTRAL CHARACTERISTICS OF Ne-LIKE IONS ON THE BASIS OF OPTIMIZED RELATIVISTIC MANY-BODY PERTURBATION THEORY

Theoretical studying spectroscopic characteristics of the Ne-like multicharged ions is carried out within the relativistic many-body perturbation theory and generalized relativistic energy approach. The zeroth approximation of the relativistic perturbation theory is provided by the optimized Dirac-Kohn-Sham ones. Optimization has been fulfilled by means of introduction of the parameter to the Kohn-Sham exchange potentials and further minimization of the gauge-non-invariant contributions into radiation width of atomic levels with using relativistic orbital set, generated by the corresponding zeroth approximation Hamiltonian.

1. Introduction

It is well known that the correct data about different radiation, energetic and spectroscopic characteristics of the multielectron atoms and multicharged ions, namely, radiative decay widths, probabilities and oscillator strengths of atomic transitions, excitation and ionization cross-sections are needed in astrophysics and laboratory, thermonuclear plasma diagnostics and in fusion research. In this light, studying the spectral characteristics of the alkali elements attracts a special interest. There have been sufficiently many reports of calculations and compilation of energies and oscillator strengths for these atoms and corresponding ions (see, for example, [1–28]). In many papers the standard Hartree-Fock, Dirac-Fock methods, model potential approach, quantum defect approximation etc in the different realizations have been used for calculating energies and oscillator strengths. However, it should be stated that for the heavy alkali atoms (such as caesium and francium and corresponding ions) and particularly for their high-excited (Rydberg) states, there is not enough precise information available in literature. 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 for 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 (RMBPT) has been earlier effectively applied to computing spectra of low-lying states for some lanthanides atoms [5-11] (see also [12-22]). We use an analogous version of the perturbation theory (PT) to study spectroscopic characteristics of some Ne-like ions.

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

As the method of computing is earlier presented in detail, here we are limited only by the key topics [5-15]. 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 [12-22]. In constructing M, the Gell-Mann and Low adiabatic formula for ΔE

is used. In contrast to the non-relativistic case, the secular matrix elements are already complex in the second order of the electrodynamical PT (first order of the interelectron interaction). Their imaginary part of ΔE is connected with the radiation decay (radiation) possibility. In this approach, the whole calculation of the energies and decay probabilities of a non-degenerate excited state is reduced to the calculation and diagonalization of the complex matrix *M*. In the papers of different authors, the $\mathrm{Re}\,\Delta E$ calculation procedure has been generalized for the case of nearly degenerate states, whose levels form a more or less compact group. One of these variants has been previously introduced: for a system with a dense energy spectrum, a group of nearly degenerate states is extracted and their matrix *M* is calculated and diagonalized. If the states are well separated in energy, the matrix *M* reduces to one term, equal to ΔE. The non-relativistic secular matrix elements are expanded in a PT series for the interelectron interaction. The complex secular matrix *M* is represented in the form [12-14]:

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

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 using Feynman diagrams (look Ref. in [1,2]). 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 take into account 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 [1,2]:

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

where $\tilde{M}^{(1)}$ is the modified one-quasiparticle matrix (diagonal), and $\tilde{M}^{(2)}$ is 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 reviews in [5-7] and 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 [3]. Glushkov-Ivanov have developed a new relativistic gauge-conserved version of the energy approach [14]. In ref. [25, 29-35] it has been developed its further generalization. Here we applied this approach for generating the optimized relativistic orbitals basis in the zeroth approximation of the many-body PT. Optimization has been fulfilled by means of introduction of the parameter to the Fock and Kohn-Sham exchange potentials and further minimization of the gauge-non-invariant contributions into radiation width of atomic levels with using relativistic orbital bases, generated by the corresponding zeroth approximation Hamiltonians. Other details can be found in Refs. [1-5,36-44].

3. Some results and conclusion

In tables 1 and 2 we present the values of probabilities of the transitions between levels of the configurations $2s^22p^53s,3d,4s,4d$ and $2s2p^63p,4p$ in the Ne-like ions of the Ni XIX, Br XXVI (in s^{-1}; total angle moment J=1): a – the MCDF method; b- relativistic PT with the empirical zeroth approximation (RPTMP); c1 – REA-PT data (without correlation corrections); c2 – REA-PT data (with an account for the correlation); exp.- experimental data (look [1-6] and Refs therein); This work -our data.

Table 1.

Probabilities of radiation transitions between levels of the configurations $2s^22p^53s,3d,4s,4d$ and $2s2p^63p,4p$ in the Ne-like ion of Ni XIX (in s^{-1}; total angle moment J=1): a – the MCDF method; b- relativistic PT with the empirical zeroth approximation (RPTMP); c1, c2 – REA PT data (without and with account for correlation effects); exp. - experiment; this work-our data (see text)

Level J=1	Exp.	a-MCDF	b-RPTMP
$2p_{3/2}3s_{1/2}$	7.6+11	9.5+11	1.3+12
$2p_{1/2}3s_{1/2}$	6.0+11	1.8+12	1.0+12
$2p_{3/2}3d_{3/2}$	1.4+11	2.2+11	1.5+11
$2p_{3/2}3d_{5/2}$	1.2+13	2.1+13	1.2+13
$2p_{1/2}3d_{3/2}$	3.2+13	4.8+13	3.6+13
$2s_{1/2}\ 3p_{1/2}$			8.5+11
$2s_{1/2}\ 3p_{3/2}$			5.1+12
$2p_{3/2}4s_{1/2}$	3.3+11		3.6+11
$2p_{1/2}4s_{1/2}$	2.0+11		3.0+11
$2p_{3/2}4d_{3/2}$	4.5+10		5.2+10
$2p_{3/2}4d_{5/2}$	8.3+12		8.3+12
$2p_{1/2}4d_{3/2}$	8.1+12		7.9+12
Level J=1	c1- REA PT	c2- REA PT	This work
$2p_{3/2}3s_{1/2}$	9.7+11	8.1+11	7.9+11
$2p_{1/2}3s_{1/2}$	7.6+11	6.2+11	6.1+11
$2p_{3/2}3d_{3/2}$	1.7+11	1.4+11	1.3+11
$2p_{3/2}3d_{5/2}$	1.5+13	1.2+13	1.1+13
$2p_{1/2}3d_{3/2}$	4.0+13	3.3+13	3.2+13
$2s_{1/2}\ 3p_{1/2}$	9.5+11	8.1+11	8.0+11
$2s_{1/2}\ 3p_{3/2}$	5.6+12	4.7+12	4.6+12
$2p_{3/2}4s_{1/2}$	4.1+11	3.4+11	3.3+11
$2p_{1/2}4s_{1/2}$	3.1+11	2.4+11	2.2+11
$2p_{3/2}4d_{3/2}$	5.4+10	4.8+10	4.6+10
$2p_{3/2}4d_{5/2}$	9.2+12	8.2+12	8.1+12
$2p_{1/2}4d_{3/2}$	8.9+12	8.0+12	8.0+12
$2s_{1/2}4p_{1/2}$	6.3+11	5.7+11	5.6+11
$2s_{1/2}4p_{3/2}$	2.7+12	2.4+12	2.3+12

Analysis of the data shows that the computational method used provides a

physically reasonable agreement between the theoretical and experimental data.

Table 2.

Probabilities of radiation transitions between levels of the configurations $2s^2 2p^5 3s,3d,4s,4d$ and $2s2p^6 3p,4p$ in the Ne-like ion of Br XXVI (in s^{-1}; total angle moment J=1): a – the DF method; b- RPTMP; c1,2 – REA PT data (without and with account for correlation effects); exp. - experiment; this -our data

Level J=1	Exp.	a-MCDF	b-RPTMP
$2p_{3/2}3s_{1/2}$	4.5+12	6.2+12	4.4+12
$2p_{1/2}3s_{1/2}$	3.1+12	4.8+12	2.8+12
$2p_{3/2}3d_{3/2}$	2.8+11	3.9+11	2.9+11
$2p_{3/2}3d_{5/2}$	6.1+13	8.0+13	6.3+13
$2p_{1/2}3d_{3/2}$	8.6+13	9.5+13	8.7+13
$2s_{1/2}\ 3p_{1/2}$	3.9+12		4.2+12
$2s_{1/2}\ 3p_{3/2}$	1.4+13		1.5+13
$2p_{3/2}4s_{1/2}$	1.1+12		1.2+12
$2p_{1/2}4s_{1/2}$	2.1+12		2.5+12
$2p_{3/2}4d_{3/2}$	2.8+10		7.3+10
$2p_{3/2}4d_{5/2}$			2.8+13
$2p_{1/2}4d_{3/2}$	2.0+13		2.2+13
$2s_{1/2}4p_{1/2}$	2.5+12		
$2s_{1/2}4p_{3/2}$	7.1+12		
Level J=1	c1-QED PT	c2-QED PT	This work
$2p_{3/2}3s_{1/2}$	5.5+12	4.4+12	4.3+12
$2p_{1/2}3s_{1/2}$	3.6+12	2.7+12	2.6+12
$2p_{3/2}3d_{3/2}$	3.5+11	2.8+11	2.7+11
$2p_{3/2}3d_{5/2}$	7.5+13	6.1+13	6.1+13
$2p_{1/2}3d_{3/2}$	9.9+13	8.6+13	8.5+13
$2s_{1/2}\ 3p_{1/2}$	4.7+12	4.0+12	3.9+12
$2s_{1/2}\ 3p_{3/2}$	1.8+13	1.4+13	1.3+13
$2p_{3/2}4s_{1/2}$	1.5+12	1.1+12	1.1+12
$2p_{1/2}4s_{1/2}$	2.8+12	2.3+12	2.2+12
$2p_{3/2}4d_{3/2}$	6.9+10	6.3+10	6.0+10
$2p_{3/2}4d_{5/2}$	2.7+13	2.3+13	2.2+13
$2p_{1/2}4d_{3/2}$	2.3+13	2.0+13	1.9+13
$2s_{1/2}4p_{1/2}$	2.9+12	2.6+12	2.5+12
$2s_{1/2}4p_{3/2}$	8.9+12	8.0+12	7.8+12

Let us note that the transition probabilities values in the different photon propagator gauges are practically equal. Besides, an account of the inter particle (electron) correlation effects is of a great importance.

References

1. Ivanova, E., Glushkov, A. Theoretical investigation of spectra of multicharged ions of F-like and Ne-like isoelectronic sequences. J. Quant. Spectr. and Rad. Tr. **1986**, *36*(2), 127-145.
2. Ivanova, E.P., Ivanov, L.N., Glushkov, A., Kramida, A. High order corrections in the relativistic perturbation theory with the model zeroth approximation, Mg-Like and Ne-Like Ions. *Phys. Scripta* **1985**, *32,* 513-522.
3. Safronova, U., Cowan, T., Safronova, M. Relativistic many-body calculations of electric-dipole lifetimes, transition rates and oscillator strengths for 2l−13l′ states in Ne-like ions. *J. Phys. B: At., Mol. and Opt. Phys*. **2005**, *38*(15), 2741–2763.
4. Glushkov, A.V., Khetselius, O.Yu., Svinarenko, A.A., Buyadzhi, V.V., *Spectroscopy of autoionization states of heavy atoms and multiply charged ions*. TEC: Odessa, **2015**.
5. Glushkov, A.V. *Relativistic Quantum theory. Quantum mechanics of atomic systems*. Astroprint: Odessa, **2008**.
6. Khetselius, O.Yu. *Hyperfine structure of atomic spectra*. Astroprint: **2008**.
7. Khetselius, O.Yu. *Quantum structure of electroweak interaction in heavy finite Fermi-systems*. Astroprint: Odessa, **2011**.
8. Glushkov, A.V. Operator Perturbation Theory for Atomic Systems in a Strong DC Electric Field. In Advances in Quantum Methods and Applications in Chemistry, Physics, and Biology. Springer: Cham, **2013,** 27, 161–177.
9. Buyadzhi, V., Zaichko P., Antoshkina, O., Kulakli T., Prepelitsa, P., Ternovsky, V., Mansarliysky V. Computing of radiation parameters for atoms and multicharged ions within relativistic energy approach:

Advanced Code. *J. Phys.: Conf. Ser*. **2017**, *905*(1), 012003.
10. Glushkov, A.V., Gurskaya, M.Yu., Ignatenko, A., Smirnov, A., Serga, I.N., Svinarenko, A., Ternovsky, E. Computational code in atomic and nuclear quantum optics: Advanced computing multiphoton resonance parameters for atoms in a strong laser field. *J. Phys: C Ser*. **2017**, *905*, 012004.
11. Svinarenko, A.A., Ternovsky, V.B., Cherkasova I., Mironenko D. Theoretical studying spectra of ytterbium atom on the basis of relativistic many-body perturbation theory: doubly excited states. *Photoelectr.* **2018**, 27, 113-120**.**
12. Ivanov, L.N., Ivanova, E.P., Knight, L. Energy approach to consistent QED theory for calculation of electron-collision strengths: Ne-like ions. *Phys. Rev. A.* **1993,** *48,* 4365-4374.
13. Glushkov, A., Ivanov, L., Ivanova, E.P. Autoionization Phenomena in Atoms. *Moscow Univ. Press*, Moscow, **1986,** 58.
14. Glushkov, A., Ivanov, L. Radiation decay of atomic states: atomic residue polarization and gauge noninvariant contributions. *Phys. Lett.A.***1992,** *170,* 33.
15. Glushkov A.V., Ivanov, L.N. DC strong-field Stark effect: consistent quantum-mechanical approach. *J. Phys. B: At. Mol. Opt. Phys.* **1993,** *26,* L379-386.
16. Glushkov, A.V. *Relativistic and Correlation Effects in Spectra of Atomic Systems*. Astroprint: **2006**.
17. Glushkov, A.V. Relativistic polarization potential of a many-electron atom. *Sov. Phys. Journal.* **1990**, *33(1)*, 1-4.
18. Glushkov, A.V. Advanced relativistic energy approach to radiative decay processes in multielectron atoms and multicharged ions. In *Quantum Systems in Chemistry and Physics*: *Progress in Methods and Applications.* Springer: Dordrecht, **2012,** 26, 231–252.
19. Glushkov, A.V. Energy approach to resonance states of compound superheavy nucleus and EPPP in heavy nuclei collisions. In Low Energy Antiproton Physics. AIP: New York, *AIP Conf. Proc*. **2005**, *796*, 206-210.
20. Glushkov, A. Spectroscopy of coope-rative muon-gamma-nuclear processes: Energy and spectral parameters *J. Phys.: Conf. Ser.* **2012,** *397,* 012011.
21. Khetselius O. Spectroscopy of cooperative electron-gamma-nuclear processes in heavy atoms: NEET effect *J. Phys.: Conf. Ser.* **2012,** *397,* 012012.
22. Glushkov, A.V. Spectroscopy of atom and nucleus in a strong laser field: Stark effect and multiphoton resonances. *J. Phys.: Conf. Ser*. **2014**, *548*, 012020
23. Glushkov, A., Svinarenko, A., Ternovsky, V., Smirnov, A., Zaichko, P. Spectroscopy of the complex auto ionization resonances in spectrum of helium. *Photoelectr*. **2015**, *24*, 94-102.
24. Glushkov, A. Multiphoton spectroscopy of atoms and nuclei in a laser field: Relativistic energy approach and radiate-on atomic lines moments method. *Adv. in Quantum Chem.* **2019**, *78*, 253-285.
25. Khetselius, O.Yu. Optimized relativistic many-body perturbation theory calculation of wavelengths and oscillator strengths for Li-like multicharged ions. Adv. Quant. Chem. **2019**, *78*, 223-251
26. Glushkov, A., Loboda, A., Gurnitskaya, E., Svinarenko, A. QED theory of radiation emission and absorption lines for atoms in a strong laser field. *Phys. Scripta.* **2009,** *T135,* 014022.
27. Florko, T.A., Tkach, T.B., Ambrosov, S.V., Svinarenko, A.A. Collisional shift of the heavy atoms hyperfine lines in an atmosphere of the inert gas. *J. Phys.: Conf. Ser*. **2012**, *397*, 012037.
28. Buyadzhi, V. Laser multiphoton spectro scopy of atom embedded in Debye plasmas: multiphoton resonances and transitions. *Photoelectr*. **2015,** *24,* 128.
29. 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, *25,* 97-101.
30. Buyadzhi, V.V., Chernyakova, Yu.G., Antoshkina, O., Tkach, T. Spectroscopy of multicharged ions in plasmas: Oscillator strengths of Be-like ion Fe. *Photoelectronics*. **2017,** *26,* 94-102.
31. Khetselius, O.Yu. Relativistic Energy Approach to Cooperative Electron-γ-Nuclear Processes: NEET Effect. In Quantum Systems in Chem. and Phys., Springer: Dordrecht, **2012,** *26,* 217-229.
32. Svinarenko, A. Study of spectra for lanthanides atoms with relativistic many-body perturbation theory: Rydberg resonances. *J. Phys.: Conf. Ser.* **2014,** *548,* 012039.
33. Khetselius, O.Yu. Relativistic perturbation theory calculation of the hyperfine structure parameters for some heavy-element isotopes. *Int. Journ. Quant. Chem.* **2009,** *109,* 3330-3335.
34. Khetselius, O.Yu. Relativistic calculation of the hyperfine structure parameters for heavy elements and laser detection of the heavy isotopes. *Phys.Scripta.* **2009,** *135,* 014023.
35. Khetselius, O. Optimized perturbation theory for calculating the hyperfine line shift and broadening of heavy atoms in a buffer gas. In *Frontiers in Quantum Methods and Applications in Chemistry and Physics*. Springer, **2015,** 29, 55-76.
36. Svinarenko, A. A., Glushkov, A. V., Khetselius, O.Yu., Ternovsky, V.B., Dubrovskaya, Yu., Kuznetsova, A., Buyadzhi, V. Theoretical spectroscopy of rare-earth elements: spectra and autoionization resonances. *Rare Earth Element* (InTech). **2017**, pp 83-104.
37. Glushkov, A.V., Khetselius, O.Yu., Svinarenko, A.A., Buyadzhi, V.V., Ternovsky, V., Kuznetsova, A.A., Bashkarev P. Relativistic perturbation theory formalism to computing spectra and radiation characteristics: application to heavy element. *Recent Studies in Perturbation Theory.* InTech. **2017**, 131.
38. Glushkov A., Svinarenko, A., Ignatenko, A.V. Spectroscopy of autoionization resonances in spectra of the lanthanides atoms. *Photoelectr*. **2011**, *20*, 90-94.
39. Dubrovskaya, Yu., Khetselius, O.Yu., Vitavetskaya, L., Ternovsky, V., Serga, I. Quantum chemistry and spectroscopy of pionic atomic systems with accounting for relativistic, radiative, and strong interaction effects. *Adv. Quantum Chem.* **2019,** *78*, 193-222.
40. Khetselius, O.Yu., Glushkov, A.V., Dubrovskaya, Yu.V., Chernyakova, Yu., Ignatenko, A., Serga, I., Vitavetskaya, L. Relativistic quantum chemistry and spectroscopy of exotic atomic systems with accounting for strong interaction effects. In *Concepts, Methods and Applications of Quantum Systems in Chem. and Phys*. Springer, **2018,** *31*, 71.
41. Ambrosov S., Ignatenko V., Korchevsky D., Kozlovskaya V. Sensing stochasticity of atomic systems in crossed electric and magnetic fields by analysis of level statistics for continuous energy spectra. *Sensor Electr. and Microsyst. Techn*. **2005**, Issue 2, 19-23.
42. Glushkov, A., Buyadzhi, V., Kvasikova, A., Ignatenko, A., Kuznetsova, A., Prepelitsa, G., Ternovsky, V. Non-linear chaotic dynamics of quantum systems: Molecules in an electromagnetic field and laser systems. In: *Quantum Systems in Phys., Chem. and Biology*. Springer, Cham. **2017**, *30*, 169-180.
43. Glushkov A., Khetselius, O., Svinarenko A. Theoretical spectroscopy of auto ionization resonances in spectra of lanthanides atoms. *Phys. Scripta*. **2013**, *T153*, 014029.
44. Glushkov A., Khetselius O., Svinarenko A, Buyadzhi V, *Methods of computational mathematics and mathematical physics. P1.* TES: Odessa, **2015.**

PACS 32.30.-r

A. V. Glushkov, I. S. Cherkasova, V. B. Ternovsky, A. A. Svinarenko

THEORETICAL STUDYING SPECTRAL CHARACTERISTICS OF Ne-LIKE IONS ON THE BASIS OF OPTIMIZED RELATIVISTIC MANY-BODY PERTURBATION THEORY

Summary. Theoretical studying spectroscopic characteristics of the Ne-like multicharged ions is carried out within the relativistic many-body perturbation theory and generalized relativistic energy approach.The zeroth approximation of the relativistic perturbation theory is provided by the optimized Dirac-Kohn-Sham ones. Optimization has been fulfilled by means of introduction of the parameter to the 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 sets, generated by the corresponding zeroth approximation Hamiltonian.

Keywords: Relativistic perturbation theory, optimized zeroth approximation, Ne-like multicharged ions

PACS 32.30.-r

А. В. Глушков, И. С. Черкасова, В. Б. Терновский, А. А. Свинаренко

ТЕОРЕТИЧЕСКОЕ ИЗУЧЕНИЕ СПЕКТРАЛЬНЫХ ХАРАКТЕРИСТИК Ne-ПОДОБНЫХ ИОНОВ НА ОСНОВЕ ОПТИМИЗИРОВАННОЙ РЕЛЯТИВИСТСКОЙ МНОГОЧАСТИЧНОЙ ТЕОРИИ ВОЗМУЩЕНИЙ

Резюме. В рамках релятивистской многочастичной теории возмущений и обобщенного релятивистского энергетического подхода проведено теоретическое изучение спектроскопических характеристик ряда Ne-подобных многозарядных ионов. В качестве нулевого приближения релятивистской теории возмущений выбрано оптимизированное приближение 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 релятивистского базиса орбиталей, сгенерированного соответствующим гамильтонианом нулевого приближения.

Ключевые слова: Релятивистская теория возмущений, оптимизированное нулевое приближение, Ne-подобные многозарядные ионы

PACS 32.30.-r

О. В. Глушков, І. С. Черкасова, В. Б. Терновський, А. А. Свинаренко

ТЕОРЕТИЧНЕ ВИВЧЕННЯ СПЕКТРАЛЬНИХ ХАРАКТЕРИСТИК Ne-ПОДІБНИХ ИОНОВ НА ОСНОВІ ОПТИМІЗОВАНОЇ РЕЛЯТИВІСТСЬКОЇ БАГАТОЧАСТКОВІ ТЕОРІЇ ЗБУРЕНЬ

Резюме. В рамках релятивістської багаточастинкової теорії збурень і узагальненого релятивістського енергетичного підходу проведено теоретичне вивчення спектроскопічних

характеристик ряду Ne-подібних багатозарядних іонів. В якості нульового наближення релятивістської теорії збурень обрано оптимізоване наближення Дірака-Кона-Шема. Оптимізація виконана шляхом введення параметра в обмінний потенціал Кона-Шема і подальшої мінімізації калібрувально-неінваріантних вкладів в радіаційні ширини атомних рівнів з використанням релятивістського базису орбіталей, згенерованого відповідним гамільтоніаном нульового наближення.

Ключові слова: Релятивістська теорія збурень, оптимізоване нульове наближення, Ne-подібні багатозарядні іони