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

A theoretical study of the spectroscopic characteristics of Zn-like multiply charged ions is carried out within the framework of the relativistic many-body perturbation theory. The optimized Dirac-Kohn-Sham approximation was chosen as the zero approximation of the relativistic perturbation theory. Optimization has been fulfilled by means of introduction of the parameters to the Kohn-Sham exchange and correlation 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. In recent years, in connection with the unprecedented progress in the development of experimental techniques, an urgent need has arisen to solve the required problems at a fundamentally new level of theoretical consistency and accuracy. First of all, this relates to the determination of such important atomic spectroscopic characteristics as the cross sections of various elementary processes, the probability of radiative transitions, and the strength of oscillators, and if important progress has been made in the study of the most intense allowed (electric dipole) radiative transitions [1–28]). In many papers the standard Hartree-Fock (HF), Dirac-Fock (DF) methods, model potential (MP) 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. 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, itera-

tions 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]). In this paper theoretical studying spectroscopic characteristics of the Zn-like multicharged ions is carried out within the relativistic many-body perturbation theory. The zeroth approximation of the relativistic perturbation theory is provided by the optimized Dirac-Coulomb one.

2. 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 [10-22]. 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 . The complex secular matrix M is represented in the form [6-11]:

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

where $M^{(0)}$ is the contribution of the vacuum diagrams of all order of PT, and $M^{(1)}$, $M^{(2)}$, $M^{(3)}$ those of the one-, two- and three-quasiparticle diagrams respectively. $M^{(0)}$ is a real matrix, proportional to the unit matrix. It determines only the general level shift. 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 $\text{Re}M^{(2)}$ 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 [4-20]. 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. Interelectron interaction operator with accounting for the Breit interaction has been taken as follows:

$$V(r_i r_j) = \exp(i\omega r_{ij}) \cdot \frac{(1 - \alpha_i \alpha_j)}{r_{ij}}, \quad (2)$$

where, as usually, α_i are the Dirac matrices.

The total probability of a λ -pole transition is the sum of the electrical P_λ^E (electric multipole decomposition) and magnetic P_λ^M (corresponding decomposition) parts and is calculated within the relativistic energy formalism [7-20]. In the energy approach with respect to the complex multielectron atomic system the energy shift in the complex form is: $\delta E = \text{Re}\delta E + i \text{Im}\delta E$, $\text{Im} \delta E = -P/2$, where P - probability of decay (transition). For a single quasiparticle atomic system $\text{Im}\delta E$ and, accordingly, P in the 2nd perturbation theory order (the perturbation operator $U_{MF}(r_i | b) - J_\mu(x)A^\mu(x)$, where A is the vector of the electromagnetic field potential, J is the current operator, U_{MF} is a mean-field potential) is proportional to the matrix element with Dirac bispinors φ_i^{EFMP} (ab initio RMP приближения):

$$V_{ijkl} = \iint d^3r_1 d^3r_2 \varphi_i^{EFMP*}(r_1) \varphi_j^{EFMP*}(r_2) [(1 - \alpha_1 \alpha_2) \cdot \sin |\omega| r_{12} / r_{12}] \cdot \varphi_k^{EFMP}(r_2) \varphi_l^{EFMP}(r_1) \quad (3)$$

which are decomposed into a series of Bessel functions of the 1st kind (analog of multipole decomposition). 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 [11] have developed a new relativistic gauge-conserved version of the energy approach. In ref. [16-28] 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. All calculations are performed with using the PC code Super atom [6-28]. The results of our studying the Zn-like ions are listed in Table 1.

Table 1.

Experimental (exp.) And theoretical energies (in atomic units) and oscillator strengths for the $4s^2(^1S_0) - 4s4p(^1P^0_1)$ transition in the spectra of various Zn-like ions: HF, DF, DF methods using experimental transition energy and our data (RPT)

Ion	Method	ΔE	f_L	f_V
Ga^+	DF	0.3351	1.89	1.98
	HF	0.2984	2.30	2.01
	DF _{exp}	0.3221	1.97	1.95
	MP	0.3076	1.68	1.73
	RPT	0.3221	1.86	1.86
	Exp.	0.3221	1.85 ± 0.15	1.85 ± 0.15
As^{3+}	DF	0.5247	1.87	1.86
	RPT	0.5140	1.57	1.57
	Exp.	0.5141	1.56 ± 0.23	1.56 ± 0.23
Yb^{40+}	DF	6.2564	1.12	1.10
	RPT	5.1788	0.97	0.96
Pb^{52+}	DF	11.1153	1.21	1.18
	RPT	10.9715	1.13	1.13
U^{62+}	DF	17.8584	1.37	1.36
	HF	17.6087	1.41	1.47
	RPT	17.6285	1.33	1.33
	Exp.	-	1.31 ± 0.05	1.31 ± 0.05

In fact in table 1 for illustration we present the experimental (exp.) and theoretical energies (in atomic units) and oscillator strengths for the $4s^2(^1S_0) - 4s4p(^1P^0_1)$ transition in the spectra of various Zn-like ions: theory is presented by the Hartree-Fock (HF) Dirac-Fock

(DF) methods plus the DF data with experimental transition energy and our data (RPT) (see [1-,5,6] and refs therein). Analysis of the data shows that the computational method used provides a physically reasonable agreement between the theoretical and experimental data. 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.

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

Summary. A theoretical study of the spectroscopic characteristics of Zn-like multiply charged ions is carried out within the framework of the relativistic many-body perturbation theory. The optimized Dirac-Kohn-Sham approximation was chosen as the zero approximation of the relativistic perturbation theory. Optimization has been fulfilled by means of introduction of the parameters to the Kohn-Sham exchange and correlation 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.

Keywords: Relativistic perturbation theory, Zn-like multicharged ions

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

Резюме. Теоретическое изучение спектроскопических характеристик Zn - подобных многозарядных ионов проводится в рамках релятивистской теории возмущений многих тел. В качестве нулевого приближения релятивистской теории возмущений выбрано оптимизированное приближение Дирака- Кона-Шема. Оптимизация выполнена путем введения параметров 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, Zn-подобные ионы

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**ТЕОРЕТИЧНЕ ВИВЧЕННЯ СПЕКТРАЛЬНИХ ХАРАКТЕРИСТИК
Ne-ПОДІБНИХ ІОНОВ НА ОСНОВІ ОПТИМІЗОВАНОЇ РЕЛЯТИВІСТСЬКОЇ
БАГАТОЧАСТКОВОЇ ТЕОРІЇ ЗБУРЕНЬ**

Резюме. Теоретичне вивчення спектроскопічних характеристик Zn - подібних багатозарядних іонів проводиться в рамках релятивістської теорії збурень багатьох тіл. 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 калібрувальних-неінваріантних вкладів в радіаційні ширини атомних рівнів з використанням релятивістського базису орбіталей, згенерованого відповідним гамільтоніаном нульового наближення.

Ключові слова: Релятивістська теорія збурень, Zn- подібні іони.