PACS 32.30.-r

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OPTIMIZED RELATIVISTIC MANY-BODY PERTURBATION THEORY IN CALCULATIONS OF ATOMIC SPECTRAL AND RADIATION CHARACTERISTICS: Eu ATOM

The new formalism of the relativistic gauge-invariant perturbation theory (RMBPT-ODF) with the optimized Dirac-Fock approximation and a generalized energy approach is applied to the study of energy, radiation, and spectroscopic characteristics of a group of heavy atomic systems, in particular, energy levels and transition probabilities and oscillator strengths of the transitions $4f^7(^8S)6s^2\ ^8S_{7/2}$ $4f^7(^8S)6s6p\ ^8P_{5/2,7.2,9.2}$, $4f^7(^8S)6s7p\ ^8P_{5/2,7\backslash 2}$, $4f^7(^8S)6s8p\ ^8P_{9/2,7\backslash 2}$ in spectrum of the europium atom Eu I. It is shown that the required formalism, in comparison with the standard non-optimized relativistic Hartree-Fock and Dirac-Fock methods, allows obtaining more accurate data both on energies and amplitudes and probabilities of radiative transitions, which is due to the use of the optimized zero ODF approximation, a fairly complete and effective account of complex many-body exchange-correlation effects. The contribution due to the polarization of the core reaches 30% of the value of the oscillator strength; the value of the calibration-invariant contribution to the radiation width is fractions of a percent, in contrast to all existing methods of modern atomic spectroscopy, for which the contribution reaches 5-50%.

1. Introduction

The study of energy, radiation, spectroscopic, and generally structural properties of heavy neutral and highly ionized atoms (so-called multiply charged ions) is of fundamental fundamental importance in many areas of atomic physics (theory of atomic spectra, spectroscopy, theory of spectral lines), astrophysics , plasma physics, laser physics, etc [1-34]. The development of new directions in the field of atomic optics and spectroscopy, laser physics and quantum electronics, such as precision spectroscopy of heavy and superheavy atoms and multi-charged ions, the latest astrophysical research, pulsed heating methods in experiments on controlled thermonuclear synthesis, the creation of fundamentally of new schemes of lasers in VUF, as well as further improvement and development of new experimental technologies, in particular with the use of new laser technologies, accelerators, etc., determines the urgent need to solve urgent and important tasks of atomic optics and laser physics on to a fundamentally new relativistic level of theoretical consistency and accuracy. In the last decade, relativistic theoretical spectroscopy of heavy both ordinary and exotic atomic systems, the so-called relativistic multi-electron and hadronic atoms, as well as heavy multi-charged ions, which covers the ultraviolet and X-ray spectrum ranges, has been actively developing. It is well known that the study of the structure of the spectral lines of such atomic systems is of great interest for the further development of atomic and nuclear theories, as well as the theory of fundamental interactions, including electroweak and strong. Experiments to determine the properties of the splitting of spectral lines, in particular, the study of the characteristics of the ultrafine structure, make it possible to specify the values of the nuclear magnetic moments of various isotopes and to check the accuracy of various computational models used for the theoretical description of atomic nuclei in heavy systems [1-25].

Most of the standard methods of the theory, despite the known progress in their development, are not able to provide a simultaneous

precise description of all the listed groups of effects and corrections. Indeed, despite numerous attempts to develop precise methods for describing the spectra of heavy atomic systems (the mega-Dirac-Fock (DF=DF) method, the R-matrix method, the relativistic coupled-cluster method, various versions of the TK etc.; packages: "SUPERSTRUCTURE", "Dirac"-package, "Beta-package", "QED", "GRASP", "BERTHA", etc.), a whole set of problems of simultaneous high-precision calculation remains unsolved above mentioned effects. Moreover, there is no information about a rather large number of particularly heavy and superheavy atoms (as well as the corresponding multicharged ions) of Mendeleev's periodic table, and the situation related to the study of the characteristics of superheavy elements has acquired a particularly crisis character due to the lack of any reliable data. A similar complex of complex theoretical problems is also observed in the relativistic spectroscopy of heavy hadronic (in particular, kaonic) multielectron atoms, for most of which no reliable spectroscopic data are given in the literature [26-29]. In our paper we present a formalism of the relativistic gauge-invariant perturbation theory (RMBPT-ODF) with the optimized Dirac-Fock (DF) approximation, which is applied to the study of energy, radiation, and spectroscopic characteristics of a group of heavy atomic systems, in particular, energy levels and transition probabilities and oscillator strengths of the transitions $4f^7(^8S)6s^2\ ^8S_{7/2}$ $4f^7(^8S)6s6p\ ^8P_{5/2,7.2,9.2}$, $4f^7(^8S)6s7p\ ^8P_{5/2,7\backslash 2}$, $4f^7(^8S)6s8p\ ^8P_{9/2,7\backslash 2}$ in spectrum of the europium atom Eu I. A generalized energy approach is used to calculate the transitions probabilities and oscillator strengths.

2. Relativistic many-body perturbation theory with optimized Dirac-Fock zeroth approximation

As the method of computing is earlier presented in detail, here we are limited only by the key topics [25-30]. The theoretical foundations of our method of combined relativistic RMBPT with optimized Dirac-Fock-Breit (ODF) zeroth approximation and generalized energy approach for consistent description and calculation of energetic, radiative, and spectroscopic characteristics of heavy multi-electron atomic systems with consistent, maximally precise consideration of relativistic, nuclear effects (including the effects of Breit-Rosenthal-Crawford-Schawlow, as well as Bohr-Weisskopf) and radiation QED corrections (including the radiative corrections for vacuum polarization, the self-energy part of the Lamb shift, as well as corrections of higher orders of PT, in particular, Källen-Sabry of order $\alpha^2(\alpha Z)$ and Wichmann-Kroll of order $\alpha(Z\alpha)^n$, etc. The starting basis for the development of our new - approach to the calculation of energy, radiation and spectroscopic characteristics of heavy atomic systems is the adiabatic formalism of Gell-Mann and Lowe and the ab initio PT formalism with using the Feynman diagram technique. The well-known S-matrix adiabatic formalism of Gell-Mann and Lowe leads to PT series on the coupling constant (in our case, the electromagnetic interaction) for shifts dE. The PT series are diagrammed in the standard way (using the usual technique of Feynman diagrams). At the same time, it is natural that new approximations in the theory of multielectron systems are conveniently formulated as methods of summarizing Feynman diagrams of a certain type.

In the theory of the relativistic atom, there is a technique related to the diagonalization of the own matrix M for calculating the energy shifts dE of the states, and the corresponding matrix elements are complex. For a multi-electron atomic system in the relativistic theory, the energy shift of the excited state is represented in the standard complex form as [1,31-35]:

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

$$\mathrm{Im}\ \Delta E = -\Gamma/2, \qquad (1б)$$

Their imaginary part of $^{\Delta E}$ =dE is connected with the radiation decay (radiation) possibility. 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 [1,31]:

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

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. The first two order corrections to $\mathrm{Re}\,M^{(2)}$ have been analyzed previously using Feynman diagrams (look Ref. in [2,3]). 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 [31-36].

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. The relativistic polarization potential [39] by Glushkov is used in our method.

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 Breit interaction has been taken as follows:

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

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 photoprocesses in the approximate calculations is a known fact and is investigated by Grant, Armstrong, Aymar and Luc-Koenig, Glushkov-Ivanov-Ivanova et al (see review in [9,32]). 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 (see review in [9]). 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 [32]. In ref. [30,35-40] 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.

The fundamental point of our approach is the selection of the optimized Dirac-Fock (ODF) potential as the zero approximation, and the procedure for constructing a one-quasiparticle representation is based on the principle of constructing optimized atomic bases in compliance with the principle of gauge invariance, in particular, by minimizing gauge-invariant contributions to the radiative widths of the levels. Here it is important to emphasize that this procedure is implemented in this approach for the first time, in contrast to alternative approaches in relativistic spectroscopy of heavy atoms and ions, where zero approximations were built: unoptimized (standard) DF, Dirac-Hartree-Slater, Dirac-Kohn-Sham (DKS), $X\alpha$, relativistic HF, Hartree-Fock-Slater, as well as model methods (model potential, pseudopotential, etc.). The function of a certain state of the system (ASF) with the total angular momentum J, with its z-projection M and parity p has the form:

$$\Psi_s(JM^p) = \sum_m c_m(s)\Phi(\gamma_m JM^p) \quad (4)$$

$$\Phi(\gamma_m JM^p) = \sum_i d_i \begin{vmatrix} \psi_1(1) & \cdots & \psi_1(N) \\ \vdots & \ddots & \vdots \\ \psi_N(1) & \cdots & \psi_N(N) \end{vmatrix} \quad (5)$$

where c - configuration mixing factors for the state s; $\Phi(\gamma_m JM^p)$ - state functions of a certain configuration, that is, the Slater determinant of 4-component Dirac bispinors; ψ_i - one-electron relativistic wave functions.

The one-electron wave function can be defined as

$$\psi = \frac{1}{r}\begin{pmatrix} P_{n,\kappa}(r)\cdot\Omega^{m_j}_{\kappa,j}(\theta,\phi) \\ iQ_{n,\kappa}(r)\cdot\Omega^{m_j}_{-\kappa,j}(\theta,\phi) \end{pmatrix} \quad (6)$$

where $\Omega^{m_j}_{\kappa,j}(\theta,\phi)$ - angular 2-component spinor, $P(r)$ and $Q(r)$ are the major and minor radial parts of the wave function, respectively. The optimization of the PT one-electron basis has been fulfilled by means of introduction of the parameter to the exchange potential 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 Hamiltonian [1,32-36]. Other details can be found in Refs. [25-47].

3. Some results and conclusion

In this subsection, we present the results of the calculation of transition energies and probabilities of some transitions in the spectrum of heavy complex atoms (of the lanthanides group) of europium Eu I.

Table 1 shows the considered transitions, as well as the corresponding wavelengths that we calculated. In the table w we present the results of our calculations (column F) of oscillator strengths of electric dipole transitions together with available experimental data (columns E1, E2). For comparison, this table also shows the calculation results (see details in [1, 4,5,48]) within the framework of the popular and well-known Coulomb approximation (columns A, B, C correspond to the calibration of the photon propagator: Coulomb Babushkin, Feynmann) [3] and the multi-configurational DF method (column D), F – RMBPT with the empirical model potential zeroth approximation; G - the results of our calculation.

Table 1. Transitions and corresponding wave-lengths (in A) in the spectrum of EuI (our data)

N	Transition
1	$4f^7(^8S)6s^2\ ^8S_{7/2} \rightarrow 4f^7(^8S)6s6p\ ^8P_{5/2}$
2	$4f^7(^8S)6s^2\ ^8S_{7/2} \rightarrow 4f^7(^8S)6s6p\ ^8P_{7/2}$
3	$4f^7(^8S)6s^2\ ^8S_{7/2} \rightarrow 4f^7(^8S)6s6p\ ^8P_{9/2}$
4	$4f^7(^8S)6s^2\ ^8S_{7/2} \rightarrow 4f^7(^8S)6s7p\ ^8P_{5/2}$
5	$4f^7(^8S)6s^2\ ^8S_{7/2} \rightarrow 4f^7(^8S)6s7p\ ^8P_{9/2}$
6	$4f^7(^8S)6s^2\ ^8S_{7/2} \rightarrow 4f^7(^8S)6s7p\ ^8P_{7/2}$
7	$4f^7(^8S)6s^2\ ^8S_{7/2} \rightarrow 4f^7(^8S)6s8p\ ^8P_{9/2}$
8	$4f^7(^8S)6s^2\ ^8S_{7/2} \rightarrow 4f^7(^8S)6s8p\ ^8P_{7/2}$
9	$4f^7(^8S)6s^2\ ^8S_{7/2} \rightarrow 4f^7(^8S)6s8p\ ^8P_{5/2}$
N	Wavelength (in A)
1	4661,77
2	4627,15
3	4592,01
4	2743,16
5	2738,48
6	2731,33
7	2471,09
8	2461,68
9	2520,45

The analysis of the obtained data allows us to conclude that, firstly, our theory is in fairly good agreement with the experiment, much better in comparison with the well-known multiconfigurational DF method, as well as with the simplified Coulomb approximation.

Secondly, as can be seen, in the Coulomb approximation, the calculation data using different calibrations of the photon propagator are quite different from each other, while in our theory the difference in the data regarding the strength of the oscillators does not exceed 0.05% (for the Coulomb calibration and the Babushkin calibration).

Thirdly, the calculation demonstrated an extremely significant quantitative contribution (up to 30%) due to the effects of interelectron correlation (polarization and shielding interactions) as effects of the second and higher orders of the PT. Finally, the analysis shows that the experimental data for the transitions $4f^7(^8S)6s^2\,^8S_{7/2} \rightarrow 4f^7(^8S)6s7p\,^8P_{9/2}$ та $4f^7(^8S)6s^2\,^8S_{7/2} \rightarrow 4f^7(^8S)6s7p\,^8P_{7/2}$, obviously contain some error that in principle, it is explained by the extremely significant complexity of studying the specified spectrum.

Table 2 Oscillator strengths of series of transitions in the spectrum of EuI atom: experiment – E1, E2; A, B, C – Coulomb approximation (data correspond to gauge of photon propagator: Coulomb, Feynman, Babushkin), D – multiconfiguration DF method, F – RMBPT with empirical model potential zeroth approximation, G – our RMBPT-ODF data

N	A	B	C	D
1	0,205	0,264	0,469	0,280
2	0,272	0,350	0,622	0,374
3	0,342	0,439	0,781	0,540
4	0,0228	0,0293	0,052	
5	0,0381			
6	0,0303			
7	0,0157			
8	0,0098			
9	0,0075			
N	E1	E2	F	G
1	0,433	0,49	0,478	0,475
2	0,588	0,59	0,591	0,589
3	0,740	0,74	0,740	0,741
4	0,012		0,015	0,014
5	0,0024		0,028	0,025
6	0,0027		0,022	0,026
7	0,0015		0,0017	0,0016
8	0,0060		0,0063	0,0062
9	0,0045		0,0049	0,0047

Key to the adequate accuracy of the description of the spectroscopic characteristics of europium is the precise consideration of relativistic, radiation and exchange-correlation effects, the use of optimized orbital bases. A comparison of our results with the data of calculations within the relativistic PT with the Dirac-Kon-Shem approximation shows that there is a certain difference in the values of energies and transition probabilities, which is indeed connected with the different degree of consideration, including exchange-correlation corrections.

The main conclusion of our calculations is that the method of relativistic many-body perturbation theory RMBPT developed by us with the optimized Dirac-Fock zeroth approximation (ODF) has a fairly high theoretical consistency and precision, and can be used for calculations of such complex systems as atoms of lanthanides, actinides, in general, heavy and superheavy atoms as well as multicharged ions.

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PACS 32.30.-r

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OPTIMIZED RELATIVISTIC MULTIPARTIC DISTURBANCE THEORY IN CALCULATIONS OF ATOMIC RADIATION AND SPECTRAL CHARACTERISTICS: Eu ATOM

Resume. The new formalism of the relativistic gauge-invariant perturbation theory (RMBPT-ODF) with the optimized Dirac-Fock approximation and a generalized energy approach is applied to the study of energy, radiation, and spectroscopic characteristics of a group of heavy atomic systems, in particular, energy levels and transition probabilities and oscillator strengths of the transitions $4f^7(^8S)6s^2\ ^8S_{7/2}$ $4f^7(^8S)6s6p\ ^8P_{5/2,7.2,9.2}$, $4f^7(^8S)6s7p\ ^8P_{5/2,7\backslash2}$, $4f^7(^8S)6s8p\ ^8P_{9/2,7\backslash2}$ in spectrum of the europium atom Eu I. It is shown that the required formalism, in comparison with the standard non-optimized Hartree-Fock and Dirac-Fock relativistic methods, allows obtaining more accurate data both on energies and amplitudes and probabilities of radiative transitions, which is due to the use of the optimized zero ODF approximation, a fairly complete and effective account of complex many-body exchange-correlation effects. The contribution due to the polarization of the core reaches 30% of the value of the oscillator strength; the value of the calibration-invariant contribution to the radiation width is fractions of a percent, in contrast to all existing methods of modern atomic spectroscopy, for which the contribution reaches 5-50%.

Key words: Relativistic theory, optimized Dirac-Fock method**,** study of energy and radiation characteristics, Eu atom

PACS 32.30.-r

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ОПТИМІЗОВАНА РЕЛЯТИВІСТСЬКА БАГАТОЧАСТИНКОВА ТЕОРІЯ ЗБУРЕНЬ В ОБЧИСЛЕННЯХ АТОМНИХ СПЕКТРАЛЬНИХ ТА РАДІАЦІЙНИХ ХАРАКТЕРИСТИК: АТОМ Eu

Резюме. Новий формалізм релятивістської калібрувально-інваріантної теорії збурень (RMBPT-ODF) з оптимізованим нульовим наближенням Дірака-Фока та узагальнений енергетичний підхід застосовано до вивчення енергетичних, радіаційних і спектроскопічних характеристик групи важких атомних систем, зокрема, енергій рівнів та ймовірностей переходів та сил осциляторів $4f^7(^8S)6s^2\ ^8S_{7/2}$ $4f^7(^8S)6s6p\ ^8P_{5/2,7.2,9.2}$, $4f^7(^8S)6s7p\ ^8P_{5/2,7\backslash2}$, $4f^7(^8S)6s8p\ ^8P_{9/2,7\backslash2}$ атому європію EuI. Показано, що шуканий формалізм у порівнянні зі стандартними неоптимізованими релятивістськими методами Хартрі-Фока та Дірака-Фока дозволяє отримати більш точні дані як по енергіях, так й амплітудам та ймовірностям радіаційних переходів, що обумовлено використанням оптимізованого нульового наближення ODF, досить повним ефективним урахуванням складних багаточастинкових обмінно-кореляційних ефектів. Внесок за рахунок поляризації остову досягає 30% від значення сили осцилятора; величина калібрувально-неінваріантного внеску в радіаційну ширину складає долі проценту на відміну від усіх існуючих методів сучасної атомної спектроскопії, для яких внесок досягає 5-50%.

Ключові слова: Релятивістська теорія, оптимізований метод Дірака-Фока, вивчення енергетичних та радіаційних характеристик, атом Eu

This article has been received in October 26, 2021