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THEORETICAL STUDYING RYDBERG STATES SPECTRUM OF THE URANIUM ATOM ON THE BASIS OF RELATIVISTIC MANY-BODY PERTURBATION THEORY

Theoretical studying spectrum of the Rydberg states for the uranium atom is carried out within the relativistic many-body perturbation theory with ab initio zeroth approximation 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

Development of new directions in the field of optics and spectroscopy, laser physics and quantum electronics, such as precision spectroscopy of heavy and ultra-heavy atoms and ions, newest astrospectroscopic studies, impulse heating methods in controlled thermonuclear synthesis spectrum, etc., necessitates the solution of urgent and important problems of atomic optics and laser spectroscopy at a fundamentally new level of theoretical sequence and fullness. In the last decade, spectroscopy of multiply charged ions, which covers the UV and X-ray bands of the spectrum, has been intensively developing. Significant progress in the development of experimental methods of research, in particular, a significant increase in the intensity and quality of laser radiation, the use of accelerators, colliders of heavy ions, sources of synchrotron radiation and, as a consequence, the possibility of precision study of increasingly energetic processes, stimulates the theories of new methods of theories calculation of their characteristics, in particular, radiation and autoionization ones. It is known that autoionization states play an essential role in various elementary atomic processes such as autoionization, selective photoionization, electron scattering at atoms, atomic and ionic atomic collisions, etc. The presence of autoionization states in ions significantly affects the nature of the spectrum of high-radiation astrophysical and laboratory plasma. Their radiation decay is accompanied by the formation of the most complex spectra of dielectronic satellites to resonant ion lines of subsequent ionization multiplicity, which contain information about the state of the plasma used for its diagnosis, as well as the study of the physical conditions in the solar corona and other astrophysical objects [1-25].

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 [9] and Refs. therein). However, one should remember about very complicated structure of spectra of the heavy atoms, including actinides, uranium, trans-uranium elements and others and necessity of correct accounting for the different correlation effects such as polarization interaction of the valent quasiparticles and their mutual screening, iterations of a mass operator etc.). One of the effective methods of studying the heavy atoms is the relativistic many-body perturbation theory (RMBPT), namely, [26-29]. It has been earlier effectively applied to computing spectra of low-lying states for some lanthanides atoms [25]

(see [26,27]). The aim of our present work is to use an analogous version of the relativistic many-body perturbation theory (PT) with an ab initio Dirac-Kohn-Sham approximation to study spectrum of autoionization states for the uranium. It is important to remind that isotope separation of atomic uranium using laser selective photoionization processes has attracted much attention now [3-6,9].

2. The 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 [26-29]. 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 [30-32]. 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 [26,27]:

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

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. 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 [2,3]). 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 [30-36]. 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.

Then the secular matrix is as follows:

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

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 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 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. 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 [26]. Other details can be found in Refs. [9,27-29,41-47].

3. Some results and conclusion

In Table 1 we present the measured [3] and calculated energies (in cm^{-1}) of the levels of the lower members of the Rydberg series of uranium $5f^3 7s2np$, counted from the level of 33083.3 cm^{-1}; excitation sequence: 6056.81 + 6030.6 + (5943-5951) Å.

Table 1.

The measured and calculated energies (in cm^{-1}) of the levels of the lower members of the Rydberg series of uranium $5f^3 7s2np$, counted from the level of 33083.3 cm^{-1}; excitation sequence: 6056.81 + 6030.6 + (5943-5951) Å

E_{exp} [3]	E_{th} [3]	E_{th} This work	n_{calc}
49885.6	49885.9	49889.7	44
49889.4	49889.5	49891.9	45
49893.0	49892.8	49894.2	46
49896.3	49895.8	49896.6	47
49898.9	49898.8	49898.8	48
49901.4	49901.4	49901.3	49
49903.9	49903.9	49903.9	50
		49906.2	51
		49908.4	52
		49910.5	53

In Table 2 we present the measured [3] and calculated energies (in cm^{-1}) of the levels of the lower members of the Rydberg uranium series $5f^3 7s^2 nf$, counted from the level 32857.449cm^{-1} ($5f^3 6d7s8s\,^7L_5^0$); excitation sequence: 6056.81+6113.89+(5862-5914) Å.

Analysis shows that the correct account for the complex many-body exchange-correlation effects plays very critical role.

It should be noted too that the data on energies of the members of the Rydberg series should

be checked and correspond to so called the smoothness test.

Table 2.

The observed and calculated energies (in cm^{-1}) of the levels of the lower members of the Rydberg uranium series $5f^3 7s^2 nf$, counted from the level 32857.449 cm-1 ($5f^3 6d7s8s\ ^7L_5^0$); excitation sequence: 6056.81 + 6113.89 + (5862-5914) Å

E_{exp} [3]	E_{th} [3]	E_{th} This	$n^*_{\exp}$	$n_{calc.}$
49765.3	49767	49765.0	15.10	20
49830.7	49824	49829.1	16.23	21
49877.8	49871	49876.5	17.24	22
49917.0	49911	49916.2	18.23	23

The detailed analysis shows that some presented (in literature) values of the Rydberg states energies do not correspond to this test and as result, there is a possibility of a jump to another Rydberg series. More detailed data of this study are presented in Ref. [45].

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Summary. Theoretical studying energies of the autoionization states for the uranium atom is carried out within the relativistic many-body perturbation theory with ab initio zeroth approximation 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 corresponding zeroth approximation Hamiltonian.

Keywords: Relativistic perturbation theory, optimized zeroth approximation, heavy atom, Rydberg states

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ТЕОРЕТИЧЕСКОЕ ИССЛЕДОВАНИЕ СПЕКТРА РИДБЕРГОВСКИХ СОСТОЯНИЙ АТОМА УРАНА НА ОСНОВЕ РЕЛЯТИВИСТСКОЙ МНОГОЧАСТИЧНОЙ ТЕОРИИ ВОЗМУЩЕНИЙ

Резюме. В рамках релятивистской многочастичной теории возмущений и обобщенного релятивистского энергетического подхода проведено теоретическое исследование спектра ридберговских состояний атома урана. 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, тяжелый атом, ридберговские состояния

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ТЕОРЕТИЧНЕ ВИВЧЕННЯ СПЕКТРУ РІДБЕРГІВСЬКИХ СТАНІВ АТОМУ УРАНА НА ОСНОВІ РЕЛЯТИВІСТСЬКОЇ БАГАТОЧАСТКОВІ ТЕОРІЇ ЗБУРЕНЬ

Резюме. В рамках релятивістської багаточастинкової теорії збурень і узагальненого релятивістського енергетичного підходу проведено теоретичне дослідження спектра автоіонізаційних станів атома урану. 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, важкий атом, рідбергівські стани