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THEORETICAL STUDYING SPECTRA OF YTTERBIUM ATOM ON THE BASIS OF RELATIVISTIC MANY-BODY PERTURBATION THEORY: DOUBLY EXCITED VALENCE STATES

Theoretical studying spectrum of doubly excited valence states of the ytterbium 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

This paper goes on our work on theoretical studying spectra and spectroscopic parameters for heavy atoms, namely, lanthanides atoms (see, for example [1-3]). It is well known 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, astro-physics, laser physics etc. (see Refs. [1-31]).

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 (RMBPT) has been earlier effectively applied to computing spectra of low-lying states for some lanthanides atoms [1] (see also [2-6]). We use an analogous version of the perturbation theory (PT) to study spectrum of doubly excited valence states of the ytterbium, however, the optimized zeroth approximation is generated within the Dirac-Kohn-Sham model.

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 [1-3]. 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 [26-30]. 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 imagi-

nary 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 . 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 [2]:

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

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 [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:

$$\rightarrow \tilde{} \qquad \tilde{} \quad , \qquad (2)$$

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:

$$V\left(r_i r_j\right) = exp\left(i\omega r_j\right) \cdot \frac{\left(1 - \acute{a}_i \acute{a}_j\right)}{r_j}, \qquad (3)$$

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 [32-40] 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 [3]. 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. [1] 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. [1-3,37-46].

3 Some illustration results and conclusion

The excited states of the ytterbium atom can be treated as the states with two-quasiparticles above the electron core [Xe]$4f^{14}$. In table 1 the energies (accounted from the Yb $4f^{14}$ core energy): of the YbI excited states with doubly excited valence shell are listed: *E1*- the EA-MMBPT data (from refs. [31]); *E2*- the RMBPT dat from [1,47]; E3 – our data.

Table 1.

Energies (in 10^2cm^{-1}) of some YbI excited states with doubly excited valence shell.

Config.	*J*	Theory			*Exp.*
		E1	*E2*	*E3*	
$6p_{1/2}^2$	0	-1067	-1064	-1062	-1062,7
$6p_{3/2}^2$	2	- 987	-1004	-1003	-1008.9
$6p_{1/2}6p_{3/2}$	1	-1054	-1050	-1049	-1049.0
$6p_{1/2}6p_{3/2}$	2	-1032	-1036	-1035	-1039.5
$5d_{3/2}^2$	2	-1034	-1032	-1030	-1010.8
$5d_{3/2}5d_{5/2}$	2	- 994	- 995	- 994	-994.6
$5d_{3/2}5d_{5/2}$	3	-1030	-1032	-1032	-1032.5

In table 2 our data listed for other similar states. All presented MMBPT, ROMBPT and our data on the energies are in the physically reasonable agreement with experimental data. However, comparison of the corresponding results for widths (will be listed in another paper) demonstrates again sufficiently large discrepancy. In our opinion, this fact is explained by insufficiently exact estimates of the radial integrals, using the non-optimized basises and some other additional calculation approximations.

Table 2.

Theoretical energies (in 10^2 cm^{-1}) of the YbI excited states with doubly excited valence shell.

Config.	*J*	*E2*	Config.	*J*	*E2*
$6p_{1/2}^2$	0	-1062	$6p_{3/2}5d_{5/2}$	3	- 961
$6p_{3/2}^2$	0	- 917	$6p_{3/2}5d_{5/2}$	4	-1060
$6p_{3/2}^2$	2	-1003	$5d_{3/2}^2$	0	- 981
$6p_{1/2}6p_{3/2}$	1	-1049	$5d_{3/2}^2$	2	-1031
$6p_{1/2}6p_{3/2}$	2	-1035	$5d_{5/2}^2$	0	- 962
$6p_{1/2}5d_{3/2}$	1	-1071	$5d_{5/2}^2$	2	- 968
$6p_{1/2}5d_{3/2}$	2	-1068	$5d_{5/2}^2$	4	- 859
$6p_{1/2}5d_{5/2}$	2	-1002	$5d_{3/2}5d_{5/2}$	1	- 981
$6p_{1/2}5d_{5/2}$	3	-1114	$5d_{3/2}5d_{5/2}$	2	- 994
$6p_{3/2}5d_{3/2}$	0	-1016	$5d_{3/2}5d_{5/2}$	3	-1031
$6p_{3/2}5d_{3/2}$	1	-1011	$5d_{3/2}5d_{5/2}$	4	-1025
$6p_{3/2}5d_{3/2}$	2	- 912	$7s_{1/2}6p_{1/2}$	0	-886
$6p_{3/2}5d_{3/2}$	3	-1034	$7s_{1/2}6p_{1/2}$	1	-885.6
$6p_{3/2}5d_{5/2}$	1	- 947	$7s_{1/2}6p_{3/2}$	1	- 849
$6p_{3/2}5d_{5/2}$	2	-1115	$7s_{1/2}6p_{3/2}$	2	-860

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Summary

Theoretical studying spectrum of doubly excited valence states of the ytterbium 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.

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ТЕОРЕТИЧЕСКОЕ ИЗУЧЕНИЕ СПЕКТРА ИТТЕРБИЯ НА ОСНОВЕ РЕЛЯТИВИСТСКОЙ МНОГОЧАСТИЧНОЙ ТЕОРИИ ВОЗМУЩЕНИЙ: ДВАЖДЫ ВОЗБУЖДЕННЫЕ ВАЛЕНТНЫЕ СОСТОЯНИЯ

Резюме

В рамках релятивистской многочастичной теории возмущений и обобщенного релятивистского энергетического подхода проведено теоретическое изучение спектра дважды возбужденных валентных состояний для атома иттербия. 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, иттербий

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ТЕОРЕТИЧНЕ ВИВЧЕННЯ СПЕКТРУ ІТЕРБІЮ НА ОСНОВІ РЕЛЯТИВІСТСЬКОЇ БАГАТОЧАСТКОВІ ТЕОРІЇ ЗБУРЕНЬ: ДВІЧІ ЗБУДЖЕНІ ВАЛЕНТНІ СТАНИ

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 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, енергії і ширини резонансів, оптимізоване нульове наближення, ітербій