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Svinarenko A.A., Nesterenko A.A.

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

THEORETICAL STUDYING SPECTRAL CHARACTERISTICS OF TM ATOM WITHIN OPTIMIZED RELATIVISTIC MANY-BODY THEORY

Theoretical studying Rydberg spectrum of complex lanthanide atom of Tm has been performed 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-Breit ones. Optimization has been fulfilled by means of introduction of the special gauge 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. The calculated energies and widths of autoionization resonant states $4f^{-1}_{j}$ 6s(J12)nsnp[J] of the Tm atom with n=25-35 are presented and compared with known theoretical results, received within other approaches. Two main types of the Rydberg autoionization resonances decay, namely, the classic Beutler-Fano decay channel and a new Ivanov et al reorientation-type decay channel ar4e studied. It is noted that, for example, for autoionization resonant states $4f^{13}_{5/2}6s_{1/2}(3)\mathrm{ns}_{1/2}[J]$ with the considered values of n, the decay of resonances occurs along both channels, and it is extremely difficult to understand a priori which of them is dominant.

1. Introduction

The development of new directions in the field of optics and spectroscopy, laser physics and quantum electronics, such as precision spectroscopy of heavy and superheavy atoms and ions, the latest astrospectroscopic research, pulse heating methods in controlled thermonuclear fusion research, the creation of fundamentally new schemes of lasers in the VHF, X-ray regions of the spectrum, etc., determines the need to solve the urgent and important tasks of atomic optics and laser spectroscopy at a fundamentally new level of theoretical consistency and accuracy. In the last decade, the spectroscopy of multi-charged ions, covering the UV and X-ray D-ranges of the spectrum, has also been intensively developed. 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, heavy ion colliders, sources of synchrotron radiation and, as a result, the possibility of a precise study of increasingly energetic processes, stimulates the development of new in the theory of heavy atoms theoretical methods of calculating their characteristics, in particular, radiation and autoionization. It is known that autoionization states (AS) play a significant role in various elementary atomic processes such as autoionization, selective photoionization, scattering of electrons on atoms, atom - and ion - atom collisions, etc. The presence of AS in ions significantly affects the characteristics of the radiation spectrum of high-temperature astrophysical and laboratory plasma. Their radiative decay is accompanied by the formation of the most complex spectra of dielectron satellites to the resonance lines of ions of the next ionization multiplicity, which contain information about the state of the plasma used for its diagnosis, as well as when studying the physical conditions in the solar corona, etc. astrophysical objects [1–28]).

In many papers the standard Hartree-Fock (HF), Dirac-Fock (DF) methods, model poten-

tial (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 (for example, such as lanthanides and actinides atoms) 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, iterations of a mass operator etc.).

In this paper we present the results of studying the spectral characteristics of various autoionization states (AS) (including narrow and abnormally narrow) in a spectrum of the Tm atom. The method of study is an accurate, ab initio method of relativistic many-body perturbation theory for three-quasi-particle atomic systems with a gauge-invariant zeroth approximation [25-30] and an energy approach, which is based on S-matrix formalism of Gell-Mann and Low [31-38]. Optimization has been fulfilled by means of introduction of the special gauge 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 [35-38]. The calculated energies and widths of autoionization resonant states $4f^{-1}_{j}$ 6s(J12)nsnp[J] of the Tm atom with n=25-35 are presented and compared with known theoretical results, received within other approaches (e.g. [2,3,18,32-34]).

2. Theoretical method

As the method of computing is earlier presented in detail, here we are limited only by the key topics [25-30]. 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 [31-38]:

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

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. 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 [28-31,35-38]. 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:

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

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 [31-42]. In the energy approach with respect to the complex multielectron atomic system the energy shift in the complex form is: δE = ReδE + i ImδE, Im δE = -P/ 2, where P- probability of decay (transition). For a single quasiparticle atomic system ImδE and, accordingly, P in the 2nd perturbation theory order (the perturbation operator$U_{MF}(r_i \vee b)$-$J_\mu(x)A^\mu(x)$, 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 наближення):

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

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 (e.g., see reviews in [2,3,18,29,30] and Refs. therein). For simplicity, it is worth to remind that an autoionization decay in the one-quaiparticle approximation can be represented as (i=l-3$\beta_1\beta_2\rightarrow\beta_3 k$, where β_i (i=l-3) described a set of quantum numbers of bound states, k -a state of free electron. Decay is possible only into the state of the continuous spectrum, which coincides in terms of parity and total moment J with the original AS. The width of the state associated with AC decay is determined by the connection with the continuum states and actually $\Gamma\infty|V(\beta_1\beta_2,\ \beta_3 k)|^2$. i.e., is proportional to matrix element of the interaction operator (2). The latter is determined by the known sum

$$Q_a=Q_a^{Qul}+Q_a^{Br} \qquad (3)$$

where respectively $Q_a^{Qul}$and Q_a^{Br} correspond to the Coulomb and Breit parts of the potential (2). These parts are expressed through the known atomic radial integrals R and known angular coefficients S. All details can be found in [2,28-38]. All calculations are performed with using the PC code Super atom [2,25-30,35].

3. The results and conclusions

The Tm spectrum is particularly complex. It is characterized by the position of the closely lying $4f^{-1}6snl$ Tm ionization limits and quite complex scheme of the autoionization decay of the $4f^{13}6snl$ Tm Rydberg states. The presence of 2 pairs of closely lying ionization limits (with vacancy states in the $4f^{14}$ core: : 4 $f_{7/2^{-1}}4f_{5/2^{-1}}$) causes 2 main types of autoionization decay [2,34]:

i). the classic Beutler-Fano decay (BFD) channel −

$4f^{-1}{}_{5/2}6s_{1/2}(J12)nl\text{-}4f^{-1}{}_{7/2}6s_{1/2}[J12']\ Tm^+ + leje,$

n>7, J12=2;3, J12'=3;4

ii). A new reorientation-type decay channel (ROD) for AS spectroscopy -

$4f^{-1}j\ 6s_{1/2}(J12)nl\text{-}4f^{-1}j6s_{1/2}[J12']Tm^+ + leje)$
n>25, J12=3, J12'=2;4 j=5/2,7/2,

Here, ROD denotes the decay of AC of the reorientation type, (BFD) is the channel of the

Beutler-Fano decay known in theory. The $4f^{-1}_{5/2}\,6s_{1/2}nl$ states are subject to both BFD and ROD decay. In contrast to BFD decay, ROD decay is a low-energy process that preserves one-electron quantum numbers of the atomic core: $4fj^{-1}$,$6s_{1/2}$. ROD decay can be either monopole or quadrupole.

Below we present the calculated energies and widths of AS $4f^{-1}_{j}\,6s(J12)nsnp[J]$ of the Tm atom with n=25-35. The obtained results are presented in tables 1-4. Table 1 shows the calculated values of the widths Γ2 (in cm^{-1}) and energies E2 (10 cm^{-1}) of the AS $4f^{13}_{7/2}6s_{1/2}(3)ns_{1/2}[J]$ of the Tm atom, for which ROD decay is the only channel of autoionization decay. For comparison, calculation data obtained by Ivanov et al. (E1,G1) [32-34] and Glushkov et al (E,G3) [2,18].

Table 1
Widths and energies of the AS $4f^{13}_{7/2}6s_{1/2}(3)ns_{1/2}[J]$ of the Tm atom

	J=5/2		
n	Γ1	Γ3	Γ2
25	1.18(-5)	1.29(-5)	1.25(-5)
26	-	-	1.13(-5)
30	5.77(-6)	6.72(-6)	6.12(-6)
33	-	-	3.79(-6)
35	-	-	3.21(-6)
	J=5/2		
n	E1	E3	E2
25	4985	4981	4983
26	-	-	4975
30	4995	4993	4994
33	-	-	4996
35	-	-	4998
	J=7/2		
n	Γ2		E2
25	1.58(-2)		4986
26	1.34(-2)		4988
30	3.98(-3)		4995
33	1.58(-2)		4998
35	3.18(-3)		5000

Table 2 shows our values of widths and energies of the AS $4f^{13}_{7/2}6s_{1/2}(3)np_j[J]$ and AS $4f^{13}_{5/2}6s_{1/2}(2)ns_{1/2}[J]$, for which the ROD is a single decay channel for AS studied.

Table 2.
Widths and energies of the AS $4f^{13}_{7/2}6s_{1/2}(3)np_j[J]$ of the Tm atom (our data)

(j,J)	(3/2,3/2)		(1/2,5/2)	
n	Γ2	E2	Γ2	E2
25	4.68(-5)	49862	1.40(-1)	49858
26	4.22(-5)	49877	1.33(-1)	49874
30	2.42(-5)	49939	1.03(-1)	49937
33	1.80(-5)	49971	7.54(-2)	49968
35	1.39(-5)	49992	5.72(-2)	49990
(j,J)	(3/2,5/2)		(1/2,7/2)	
n	Γ2	E2	Γ2	E2
25	1.92(-1)	49865	3.72(-2)	49848
26	1.75(-1)	48979	3.45(-2)	49863
30	1.07(-1)	49941	2.38(-2)	49938
33	8.20(-2)	49972	2/12(-2)	49961
35	6.59(02)	49993	1.76(-2)	49982
(j,J)	(3/2,7/2)		(3/2,9/2)	
n	Γ2	E2	Γ2	E2
25	3.46(-1)	49867	3.98(-1)	49869
26	3.24(-1)	49884	3.71(-1)	49886
30	2.38(-1)	49952	2.62(-1)	49953
33	2.05(-1)	49977	2.26(-1)	49978
35	1.56(-1)	49992	1.729(-1)	49993

Table 3 shows our values of widths and energies (in cm^{-1}) of the $4f^{13}_{5/2}6s_{1/2}(2)ns_{1/2}[J]$ AS.

Table 3.
Widths and energies of the AS $4f^{13}_{5/2}6s_{1/2}(2)ns_{1/2}[J]$ of the Tm atom (our data)

	J=3/2	J=3/2
n	Γ2	E2
25	2.64(-5)	5836
30	1.27(-5)	5845
35	8.89(-6)	5850
	J=5/2	J=5/2
n	Γ2	E2
25	5.32(-5)	5838
30	2.78(-5)	5846
35	1.54(-5)	5852

Analysis of the data shows that the computational method used provides a physically reasonable agreement between the theoretical and experimental data. However, comparison of the corresponding results for widths 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 4 shows the calculated widths and energies of the $4f^{13}_{5/2}6s_{1/2}(3)ns_{1/2}[J]$, states, for which autoionization decay can pass through both channels: ROD and BFD.

Table 4. Widths and energies of the AS $4f^{13}_{5/2}6s_{1/2}(3)ns_{1/2}[J]$ of the Tm atom (our data)

	Γ2 J=5/2		Γ2 J=7/2	
n	Γ(ROD)	Γ(BFD)	Γ(ROD)	Γ(BFD)
25	1.39(-2)	2.85(-5)	1.36(-5)	5.41(-5)
30	3.32(-3)	1.52(-5)	6.81(-6)	2.78(-5)
35	1.01(-3)	8.68(-6)	3.53(-6)	1.56(-5)

It is important to note that for AS $4f^{13}_{5/2}6s_{1/2}(3)ns_{1/2}[J]$ (table 4) with the considered values of n, the decay of resonances occurs along both channels, and it is extremely difficult to understand a priori which of them is dominant.

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Keywords: Relativistic perturbation theory, optimized zeroth approximation, spectroscopy, Tm atom

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Свинаренко А.А., Нестеренко А.А.

ТЕОРЕТИЧНЕ ВИВЧЕННЯ СПЕКТРАЛЬНИХ ХАРАКТЕРИСТИК Tm-АТОМА НА ОСНОВІ ОПТИМІЗОВАНОЇ РЕЛЯТИВІСТСЬКОЇ ТЕОРІЇ

Резюме. Теоретичне дослідження рідбергівського спектру складного атома (з лантаноідів) Tm виконано в рамках оптимізованої релятивістської багаточастинкової теорії збурень і узагальненого релятивістського енергетичного підходу. Нульове наближення релятивістської теорії збурень визначається оптимізованим наближенням Дірака-Кона-Шам-Брейта. Оптимізацію виконано шляхом введення спеціального калібрувального параметра до обмінних потенціалів Фока та Кона-Шема та подальшої мінімізації калібрувально-неінваріантних внесків в радіаційну ширину атомних рівнів з використанням релятивістських орбітальних наборів, породжених відповідним гамільтоніаном нульового наближення. Наведено розраховані енергії та ширини автоіонізаційних станів $4f^{-1}_j$ 6s(J12)nsnp[J] атома Tm з головним квантовим числом n=25-35 та порівняно з відомими теоретичними результатами, отриманими в рамках інших підходів. Досліджено два основних типи розпаду рідбергівських автоіонізаційних резонансів, а саме, класичний канал розпаду Бейтлера-Фано та новий канал розпаду реорієнтаційного типу, відкритий Івановим-Летоховим та інш. Зазначено, що, наприклад, для автоіонізаційних резонансів з розглянутими значеннями n розпад резонансів відбувається по обох каналах, і апріорі зрозуміти, який з них є домінуючим, надзвичайно важко.

Ключові слова: релятивістська теорія збурень, оптимізоване нульове наближення, спектроскопія, атом Tm

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