Advanced computational approach to studying Rydberg and autoionization resonances in spectra of lanthanides: Ytterbium

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Abstract. We present the results of computing the Rydberg autoionization resonances in spectra of the ytterbium atom, in particular, data on the energies and widths of the autoionization resonances \(4f^{13}[\text{F}_2]6s^2np[5/2]_2\), \(4f^{13}[\text{F}_2]6s^2n\ell[5/2]_2\), which are arisen in result of excitation of the 4f-shell electrons. For some values of the principal quantum number the presented data are compared with the corresponding available experimental data by Jong-Hoon Yi et al, which are obtained by method of three-photon laser polarization spectroscopy. As the method of computing we apply the method of a relativistic many-body perturbation theory with the Dirac-Kohn-Sham zeroth approximation combined with the generalized relativistic energy approach. This approach takes effectively into account the important exchange-correlation corrections as the corrections of the perturbation theory second and higher orders (for example, the polarization interaction, quasiparticles screening corrections) and effect of the non-Coulomb grouping levels in the Rydberg spectra etc.

1. Introduction
The intensive experimental and theoretical investigations in the field of astrophysical analysis, laboratory, thermonuclear plasma diagnostics, fusion research etc stimulate a great traditional interest to accurate computing the spectra, radiative and autoionization decay characteristics of the Rydberg atomic (atoms in the highly excited states with large values of the principal quantum number \(n \gg 1\)) systems (see, for example [1-10]). It is also provided by a great number of different important applications in laser physics and quantum electronics. For example, it is worth to mention new possible lasing generation schemes in the short-wave range with using the Rydberg systems, different topics of atomic and molecular optics and spectroscopy, quantum informatics and computing etc. At last, it is also important to remind about such unique and interesting nonlinear optical phenomena such as the Bose-condensate in vapors of the Rydberg alkali-metal atoms, the Rydberg matter, fountains of the cold Rydberg atoms, atomic (nuclear) clocks etc. At present time the Rydberg atoms and ions of relatively light elements are intensively and quite adequately studied, however, the situation became more dramatic for the Rydberg atoms and ions of the heavy and superheavy elements.

Over the last several decades, a large number of theoretical studies of atomic structure has been performed using the traditional comprehensive methods such as the well-known Hartree-Fock (HF) and Dirac-Fock (DF) methods in different versions, methods of the many-body perturbation theory (PT) with the HF and DF zeroth approximations, density functional theory, R-matrix, coupled-cluster theories, and more simplified approaches such as the quantum defect and Coulomb approximations, pseudo- and model potential methods, the classical and quasiclassical models and many others (see,
for example, [6-21] and Refs. therein). These methods have been successfully used in computing the spectroscopic properties of different light and middle Rydberg atoms. In a case of the heavy Rydberg atoms in a free state or in an external electromagnetic field a modern level of description of the Rydberg atoms is not sufficiently satisfactory. A precise accounting for the relativistic and exchange-correlation effects, including an effect of the non-Coulomb grouping levels in the Rydberg spectra (the effect, which, as a rule, is not correctly treated within simplified Coulomb and quantum defect models) is of a great interest and importance [6,8-10].

This paper is devoted to theoretical studying the Rydberg autoionization resonances in spectra of heavy elements, namely, the ytterbium atom. The ytterbium atom as the other lanthanides elements is intensively studied [22-36], nevertheless, for example, the most accurate data on spectral characteristics of the Rydberg states are absent hitherto.

As the method of computing the autoionization resonances spectra we apply the method of formally exact relativistic many-body perturbation theory with the Dirac-Kohn-Sham (DKS) zeroth approximation combined with a generalized energy approach (version [37-45]). This approach allows to take effectively into account the exchange-correlation corrections of the perturbation theory second order and higher orders (polarization interaction, quasiparticles screening, etc.). The wave function zeroth basis is found from the Dirac equation with ab initio potential, which includes the optimized Dirac-Kohn-Sham potential. The correlation corrections of the PT high orders are taken into account within the Green functions method with using the Feynman diagram’s technique. These corrections correspond to the effects of electron screening, particle-hole interactions, mass operator iterations etc. It is important to note that the method is constructed on the base of the same ideas as the well-known formalism of the PT with the model potential zeroth approximation by Ivanov-Ivanova et al [33-35,46-50]. However, there are two key differences; namely, the PT zeroth approximation [20,64-70] is the Dirac-Kohn-Sham one. In order to calculate the radiative transition and autoionization resonances parameters a new version of relativistic energy approach is used. It generalizes the known model relativistic energy approach in a case of the multielectron atom that has been proposed by Ivanov-Ivanova et al [34-36, 50-52]. A generalized gauge-invariant relativistic energy approach in a case of the multielectron atomic systems has been developed by Glushkov-Ivanov-Ivanova et al [52-60].

We present the results of the test computing energies and widths of the excited (autoionization) states for the Yb 7s6p configuration and compare these data with the available experimental (approximation) and theoretical data, obtained within different theoretical approaches such as multiconfiguration DF method, the relativistic many-body PT with the model potential zeroth approximation by Ivanov-Ivanova et al [33,34,49,50]. For the first time we list our theoretical data on the energies and widths of the autoionization resonances 4f13[7F2]6snp[5/2], 4f14[7F2]6s2nf[5/2], and compare these data with the corresponding available experimental data by Jong-hoon Yi et al [31,32].

2. Relativistic energy approach and optimized relativistic many-body perturbation theory

The method is based on the convenient field procedure, which includes computing the energy shifts $\Delta E$ of the degenerate electron states. More exactly, speech is about constructing secular matrix $M$ (with using the Gell-Mann and Low adiabatic formula for $\Delta E$), which is already complex in the relativistic theory, and its further diagonalization. It allows to compute the energies and decay probabilities of a non-degenerate excited state for a complex atomic system [46-50]. The secular matrix elements can be further expanded into a PT series on the interparticle interaction. Further the standard Feynman diagrammatic technique is usually used. Generally speaking, the secular matrix $M$ can be represented as follows:

$$M = M^{(0)} + M^{(1)} + M^{(2)} + M^{(3)},$$

where $M^{(0)}$ is the contribution of the vacuum diagrams of all PT orders (this contribution determines only the general levels spectrum shift); $M^{(1)}, M^{(2)}, M^{(3)}$ are contributions of the 1-, 2- and 3-
quasiparticle (QP) diagrams respectively. The matrix \( M^{(1)} \) can be presented as a sum of the independent one-QP contributions. Substituting these quantities into (1) one could have summarized all the one-QP diagrams contributions. In the empirical methods here the experimental values of one-electron energies are usually used, however, the necessary experimental quantities (especially for the rare-earth and other elements) are not often available. The detailed procedure for computing \( \text{Re} M^{(3)} \) is presented, for example, in Refs. [9,33-36,46-50].

The relativistic Dirac Hamiltonian of an atomic multielectron system is as follows (the atomic units are used) [9]:

\[
H = \sum_i (\alpha p_i - \beta c^2 - Z/r_i) + \sum_{i>j} \exp(i|\omega|r_{ij})(1-\alpha_i\alpha_j)/r_{ij}
\]

(2)

where \( Z \) is a charge of nucleus, \( \alpha_i, \alpha_j \) are the Dirac matrices, \( \omega \) is the transition frequency, \( c \) – the velocity of light.

The interelectron interaction potential (second term in (3)) takes into account the retarding effect and magnetic Breit interaction in the lowest order on parameter of the fine structure constant \( \alpha \). In the PT zeroth approximation we used the following mean-field potential:

\[
V_{MF} = V^{DKS}(r) = [V^D_{Coul}(r) + V_X(r) + V_C(r, a)]
\]

(3)

with the standard Coulomb \( V^D_{Coul} \), generalized exchange \( V_X \) and correlation \( V_C \) potentials [15-18]. In particular, the Kohn-Sham exchange potential looks as [15,16]:

\[
V_X[\rho(r), r] = V^{KS}_X(r) \cdot \left\{ \frac{3}{2} \ln \left[ \frac{\beta + (\beta^2 + 1)^{1/2}}{\beta(\beta^2 + 1)^{1/2}} \right] - \frac{1}{2} \right\}
\]

(4)

where \( \beta = [3\pi^2 \rho(r)]^{1/3} / c \). The corresponding generalized Lundqvist-Gunnarsson correlation potential is as follows [17,18]:

\[
V_C[\rho(r), r] = -0.0333 \cdot b \cdot \ln[1 + 18.3768 \cdot \rho(r)^{1/3}],
\]

(5)

where \( b \) is the optimization parameter [53].

The most complicated problem of the relativistic PT computing the rare-earth elements spectra is in an accurate, precise accounting for the multi-electron exchange-correlation effects (including polarization and screening effects, a continuum pressure etc), which can be treated as the effects of the PT second and higher orders. Using the standard Feynman diagrammatic technique one should analyze two kinds of diagrams (the polarization and ladder ones), which describe the polarization and screening exchange-correlation effects. The detailed description of the polarization diagrams and the corresponding analytical expressions for matrix elements of the polarization QPs interaction (through the polarizable core) potential is presented, for example, in Refs. [42-44,61-66]. An effective approach to accounting for the multi-electron polarization contributions is described earlier and based on using the effective relativistic two-quasiparticle polarizable operator [61] (generalization of the nonrelativistic operator [50]), which is included into the PT first order matrix elements.

It is important to remind that in the QED theory, the photon propagator \( D(12) \) plays the role of the interelectron interaction (look Eq.(1)) Naturally the analytical form of \( D(12) \) depends on the gauge, in which the electrodynamical potentials are written. The gauge dependence of the radiative amplitudes in the approximate calculations is a well known fact and is in details investigated by Grant, Armstrong, Aymar and Luc-Koenig, Ivanov-Ivanova-Glushkov et al (see [2-5,17,18,34-36,52-60] and Refs. therein). Grant has investigated the gauge connection with the limiting non-relativistic form of the transition operator and formulated the conditions for approximate functions of the states, in which
the amplitudes of the photo processes are gauge invariant. Glushkov-Ivanov developed a new procedure of the accurate treating the PT lowest order multielectron effects, in particular, the gauge dependent radiative contribution for the certain class of the photon propagator gauge [52,53]. The corresponding contribution is considered to be the typical representative of the important multielectron exchange-correlation effects, whose minimization is a reasonable criteria in the searching for the optimal PT one-QP basis.

Below we will be interested by studying the spectra of the autoionization resonances in the ytterbium atom and calculating their energies and widths. Usually the excited states of the ytterbium atom can be treated as the states with the 2-QP (also 3-QP) above the electron core [Xe]4f\textsuperscript{14}. Within the energy approach [33,34,50-53] the radiative and autoionization widths are determined by the square of an electron interaction matrix element having the form:

\[ V_{1234} = [(j_1 j_2 j_3 j_4)]^{1/2} \sum_{j_\mu} (-1)^{j_\mu} (j_1 j_3 j_\mu \mu) \times Q_\lambda \{1234\}, \]  

(6)

\[ Q_\lambda = Q_\text{Coul}^\lambda + Q_\text{Br}^\lambda, \]

where \( j_\mu \) is the total single electron momentums, \( m_\mu \) – the projections; \( Q_\text{Coul}^\lambda \) is the Coulomb part of interaction, \( Q_\text{Br}^\lambda \) - the Breit part. For example, the Coulomb part \( Q_\text{Coul}^\lambda \) can be expressed in terms of the known radial integrals \( R_\lambda \) and angular coefficients \( S_\lambda \) [46-50]:

\[ Q_\text{Coul}^\lambda \{1243\} = \{R_\lambda \{1243\} \} S_\lambda \{1243\} + \{R_\lambda \{1243\} \} S_\lambda \{1243\} + \{R_\lambda \{1243\} \} S_\lambda \{1243\} \]

(7)

The tilde in (7) designates that the large component of radial part of the one-QP Dirac function \( f \) must be replaced by the small one \( g \). Below is given the example of the radial integral [4,62]:

\[ R_\lambda \{1243\} = \int dr_1 r_1^2 f_1(r_1) f_2(r_1) f_3(r_1) f_4(r_1) Z^{(1)}(r_1) Z^{(1)}(r_2). \]  

(8)

where the function \( Z \) is connected with the standard Bessel functions as:

\[ Z^{(\lambda)}(r) = \frac{2}{|\alpha\lambda|} J_{\lambda + \frac{1}{2}}(\alpha |\lambda| r) r^{\lambda + \frac{1}{2}}. \]  

(9)

The angular coefficients are defined by standard way [50]. The Breit part of \( Q \) is defined in the similar way as above, but the contribution of our interest is a real part. According to the Ivanov-Ivanov et al method [34,35,46, 50,51], calculation of the integrals of the type (9) \( R_\lambda \{1243\} \) is reduced to the solution of a system of differential equations:

\[ \begin{cases} 
  y_1' = f_1 f_3 Z^{(1)}(\alpha |\lambda| r)^{2+\lambda}, \\
  y_2' = f_2 f_4 Z^{(1)}(\alpha |\lambda| r)^{2+\lambda}, \\
  y_3' = [y_1 f_2 f_4 + y_2 f_1 f_3] Z^{(2)}(\alpha |\lambda| r)^{1-\lambda}.
\end{cases} \]  

(10)

In addition it is easily to show that

\[ y_3(x) = \text{Re} R_\lambda \{1243\}, \quad y_3(x) = X_\lambda \{13\}. \]  

(11)
The system of differential equations includes also equations for functions $f^{r_{1\alpha}} \langle \alpha' \| \beta \rangle$, $g^{r_{2\alpha}} \langle \alpha' \| \beta \rangle$, $Z^{(1)}_{\alpha \beta}$, $Z^{(2)}_{\alpha \beta}$. The formulas for the autoionization (Auger) decay probability include the radial integrals $R_\alpha(\alpha \| \beta \| \gamma)$, where one of the functions describes electron in the continuum state. When calculating this integral, the correctly normalized function should be used. It is important also to note that the calculation is carried out in the $jj$-coupling scheme representation. The transition to the intermediate coupling scheme has been realized by diagonalization of the secular matrix. Indeed, only $Re M$ should be diagonalized. The imaginary part is converted by means of the matrix of eigenvectors $\{C_{\alpha \beta}\}$, obtained by diagonalization of $Re M : Im M_{\alpha \beta} = \sum_q C_{\alpha q}^* M_{qj} C_{\beta j}$; $M_{qj}$ are the matrix elements in the $jj$-coupling scheme, and $M_{\alpha \beta}$ in the intermediate coupling scheme representation. This procedure is correct to terms of the order of $Im M/Re M$ [26]. In order to reach the corresponding optimization of the relativistic wave functions, we have used the procedure [53], which derives an undoubted profit in the routine many-body calculations as it provides the way of the refinement of the atomic characteristics calculations, based on the "first principles". All computing was performed using the modified PC code “Superatom-ISAN” (version 93). Other details can be found in Refs. [9,37-50].

3. Some results and conclusions

Below we present the results for some Rydberg autoionization resonances in the spectrum of Yb. As illustration, in table 1 we present the test data of our computing energies (E4) and widths ($\Gamma$4) of the excited (autoionization) states of the YbI 7s6p configuration (accounted from the ground state: 4f$^{14}$6s$^2$ 1S0, Yb). For comparison in table 1 we also list the experimental (Letokhov et al) and theoretical data [9,22,27-29,33,34]: E1,$\Gamma$- PT with the model potential zeroth approximation by Ivanov et al [33]; E2,$\Gamma$- the optimized PT with the DF zeroth approximation [28]; E3- multiconfiguration DF method of Ref. [27] (the classification in [27] differ from Ref. [28,33]).

| Term | Theory E3 | Theory E1 | Theory $\Gamma$1 | Theory $\Gamma$2 | Theory E4 | Theory $\Gamma$4 | Exp. $\Gamma_{exp}$ | Exp. $\Gamma_{exp}$ |
|------|-----------|-----------|-----------------|-----------------|-----------|-----------------|--------------------|--------------------|
| $2^3P_0^0$ | 6123 | 5980 | 0.7 | 1.25 | 5940 | 1.20 | 5913 | 1.1 |
| $2^1P_1^0$ | 6208 | 6000 | 3.0 | 1.10 | 6205 | 1.06 | 6042 | 0.95 |
| $2^3P_0^2$ | 6242 | 6260 | 0.7 | 1.51 | 6258 | 1.54 | 6252 | 1.6 |
| $1^1P_1^0$ | 6422 | 6360 | 1.8 | 2.48 | 6370 | 2.50 | 6366 | 2.6 |

An analysis of the presented data shows physically reasonable agreement between the values of energies E1-E4 and $\Gamma_{exp}$, however, the theoretical and experimental values of the widths significantly differ. The reason of difference is explained by insufficiently exact estimate of the radial integrals, using the non-optimized bases and some other additional calculation approximations [9,17,18,28-34]. Besides, one should take into account for the important multi-body exchange-correlation effects.

In tables 2,3 we list our data on the energies ($E_\alpha$) and widths ($\Gamma_\alpha$) of the autoionization resonances 4f$^{14}$ [$^3F_{72}$]6s$^2$np[5/2], 4f$^{14}$ [$^1F_{72}$]6s$^2$nf[5/2], which are arisen in result of excitation of the 4f-shell electrons. For some values of the principal quantum number the presented data are compared with the corresponding available experimental data by Jong-hoon Yi et al, which are obtained by method of three-photon laser polarization spectroscopy [31,32]. Let us note that the obtained results are in a physically reasonable agreement with experimental data. Secondly, an accurate account for the exchange –correlation effects, including an effect of the non-Coulomb grouping levels in the Rydberg spectra plays a principally critical role. Moreover, as the detailed analysis shows, the difference between theoretical and experimental values on widths can reach a few times. It is important to note that the widths of the studied Rydberg resonances are very little.
Table 2. Energies (10 cm\(^{-1}\)) and widths (cm\(^{-1}\)) of the Yb autoionization resonances 4f\(^{13}\) [2F\(^{7/2}\)]6s\(^{2}\)np\(^{5/2}\)\(^{2}\) (see text)

| N  | \(E_{\text{exp}}\) | \(\Gamma_{\text{exp}}\) | \(E_{\text{th}}\) | \(\Gamma_{\text{th}}\) |
|----|-----------------|-----------------|-----------------|-----------------|
| 12  | 7012            | 1.5             | 7012            | 1.7             |
| 13  | 7048            | 0.4             | 7043            | 0.5             |
| 15  | 7091            | 1.2             | 7092            | 1.4             |
| 20  | 7143            | 0.6             | 7143            | 0.7             |
| 25  | 7161            | 1.3             | 7161            | 1.5             |
| 26  | 7163            | 0.6             | 7163            | 0.8             |
| 30  | 7170            | 0.5             | 7169            | 0.7             |
| 31  | 7171            | 0.4             | 7171            | 0.5             |
| 33  | 7173            | 0.6             | 7173            | 0.6             |
| 34  | -               | -               | 7174            | 0.3             |
| 35  | -               | -               | 7175            | 0.5             |
| 46  | -               | -               | 7180            | 0.4             |

Table 3. Energies (cm\(^{-1}\)) and widths (cm\(^{-1}\)) of the Yb autoionization resonances 4f\(^{13}\) [2F\(^{7/2}\)]6s\(^{2}\)nf\(^{5/2}\)\(^{2}\) (see text)

| n  | \(E_{\text{exp}}\) | \(\Gamma_{\text{exp}}\) | \(E_{\text{th}}\) | \(\Gamma_{\text{th}}\) |
|----|-----------------|-----------------|-----------------|-----------------|
| 12  | 7096            | 0.5             | 7096            | 0.7             |
| 13  | 7110            | 0.4             | 7111            | 0.5             |
| 15  | 7131            | 1.4             | 7131            | 1.6             |
| 20  | 7156            | 0.8             | 7156            | 0.9             |
| 25  | 7167            | 0.5             | 7167            | 0.8             |
| 26  | 7169            | 0.5             | 7169            | 0.7             |
| 30  | 7173            | 0.4             | 7173            | 0.5             |
| 31  | 7174            | 0.5             | 7174            | 0.6             |
| 33  | -               | -               | 7175            | 0.4             |
| 34  | -               | -               | 7176            | 0.8             |
| 35  | -               | -               | 7177            | 0.5             |
| 46  | -               | -               | 7181            | 0.3             |

This may be connected with a complex energetics of the studied atom [24-26,48]. It provides an unusual physics of autoionization resonances in spectra of the lanthanides atoms and their decay mechanisms, especially in comparison with the conventional standards of spectroscopy of the inert gases, alkali and alkaline-earth atoms (the typical resonance widths are of tens and hundreds of cm\(^{-1}\)). Speech is about the possible unusual features in behaviour of the autoionization resonances of the lanthanides atoms in a sufficiently weak dc electric (or laser) field that can be detected by a laser spectroscopy methods [9,34,78,79]. One should consider different types of autoionization decay for the lanthanides (and possibly actinides) atoms, in particular, the well known classical Beutler-Fano decay channel and additional the re-orientation type decay channel, predicted by Ivanov et al [33-36,79]. Resonances of the opposite parity are mixed with each other in a sufficiently weak DC electric (laser) field. In case of the heavy lanthanides atoms it results in new effect of the giant broadening some resonances with the little width. For the first time, for Tm, the possibility of such an effect has been predicted by Glushkov-Ivanova-Ivanov [52,79]. These interesting spectral features of the Rydberg autoionization resonances can be used in the effective selective photo-ionization schemes of separating heavy isotopes and some other important applications [1-4,67-80].
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