# Computing of radiation parameters for atoms and multicharged ions within relativistic energy approach: Advanced Code



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# Computing of radiation parameters for atoms and multicharged ions within relativistic energy approach: Advanced Code

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**Abstract.** The advanced numerical atomic code based on the combined relativistic energy approach and relativistic many-body perturbation theory with the optimized zeroth ab initio model potential approximation is presented and used in computing the radiation characteristics of the multielectron atoms and multicharged ions. There are presented the results of computing the energy levels and oscillator strengths (reduced dipole matrix elements) and lifetimes for heavy alkali atom of the caesium, in particular, there are listed data for the 7s1/2 – np1/2,3/2 (n=7-10) transitions and some Ne-like multicharged ions. The comparison of the calculated values with available theoretical and experimental (compillated) data is performed.

## 1. Introduction

It is well known that the correct data about different radiation, energetic and spectroscopic characteristics of the multielectron atoms and multicharged ions, namely, radiative decay widths, probabilities and oscillator strengths of atomic transitions, excitation and ionization cross-sections are needed in astrophysics and laboratory, thermonuclear plasma diagnostics and in fusion research. In this light, a special interest attracts studying the spectral characteristics of the alkali elements. There have been sufficiently many reports of calculations and compilation of energies and oscillator strengths for these atoms and corresponding ions (see, for example, [1–28]). In many papers the standard Hartree-Fock, Dirac-Fock methods, model potential 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 (such as caesium and francium and corresponding ions) and particularly for their high-excited (Rydberg) states, there is not enough precise information available in literatures.

This work goes on our studying the spectroscopic properties of the neutral and highly ionized atoms, which has a fundamental importance in many fields of atomic physics (spectroscopy, spectral lines theory), astrophysics, plasma physics, laser physics and so on. In this paper the combined generalized relativistic energy approach [1-4,11-14] and relativistic many-body perturbation theory with the zeroth order ab initio model potential optimized one-particle representation [1,5,13-16] are used for computing the energy levels and oscillator strengths (reduced dipole matrix elements) of radiative transitions in some heavy multielectron atoms and multicharged ions, in particular, the alkali atoms and ions and the Ne-like multicharged ions. The comparison of the calculated dipole matrix

elements with available theoretical and experimental (compillated) data is performed. A generalized relativistic energy approach to computing the radiative decay characteristics for atoms and multicharged is based on the Gell-Mann and Low adiabatic S- formalism. Originally the energy approach to radiative and autoionization processes in multielectron atoms and ions has been developed by Ivanova-Ivanov et al [22-27] (the PC code "Superatom-ISAN"). More advanced version of the relativistic energy approach has been developed in Refs. [28-32]. Different advanced computational generalizations have been considered in Refs. [33-50].

## 2. The theoretical method

In the relativistic energy approach (REA) [22-24,30] an imaginary part of the electron energy shift of an atom is directly connected with a radiation decay possibility (transition probability). An approach, is based on the Gell-Mann and Low formula with the QED scattering matrix. The total energy shift of the state in relativistic atom can be presented in the standard form:

$$\Delta E = \mathrm{Re}\Delta E + i\,\Gamma/2 \tag{1}$$

where Γ is interpreted as the level width, and the transition probability P = Γ. An imaginary part of electron energy can be defined in the lowest order of the perturbation theory as [22]:

$$\mathrm{Im}\Delta E(B) = -\frac{e^2}{4\pi} \sum_{\substack{\alpha>n>f \\ [\alpha<n\le f]}} V^{|\omega_{\alpha n}|}_{\alpha n \alpha n}, \tag{2}$$

where (α>n>f) for electron and (α<n<f) for vacancy. The matrix element is determined as follows:

$$V^{|\omega|}_{ijkl} = \iint dr_1 dr_2 \Psi^*_i(r_1)\Psi^*_j(r_2)\frac{\sin|\omega|r_{12}}{r_{12}}(1-\alpha_1\alpha_2)\Psi^*_k(r_2)\Psi^*_l(r_1) \tag{3}$$

The separated terms of the sum (3) represent the contributions of different channels; for example, a probability of the dipole transition is as follows:

$$\Gamma_{\alpha_n} = \frac{1}{4\pi}\cdot V^{|\omega_{\alpha_n}|}_{\alpha_n\alpha_n} \tag{4}$$

When calculating the matrix elements (8), one should use the angle symmetry of the task and write the corresponding expansion for $\sin|\omega|r_{12}/r_{12}$ on spherical harmonics as follows [1,24]:

$$\frac{\mathbf{sin}|\omega|r_{12}}{r_{12}} = \frac{\pi}{2\sqrt{r_1 r_2}}\sum_{\lambda=0}^{\infty}(\lambda)J_{\lambda+1/2}(|\omega|r_1)J_{\lambda+1/2}(|\omega|r_2)P_\lambda(\mathbf{cos}\,\widehat{\boldsymbol{r}_1\boldsymbol{r}_2}), \tag{5}$$

where $J$ is the Bessel function of first kind and (λ)= 2λ + 1. This expansion is corresponding to usual multipole one for probability of radiative decay. Substitution of the expansion (5) to matrix element of interaction gives as follows [24,27]:

$$V^{\omega}_{1234} = [(j_1)(j_2)(j_3)(j_4)]^{1/2}\sum_{\lambda\mu}(-1)^{\mu}\begin{pmatrix} j_1 j_3 & \lambda \\ m_1 - m_3 & \mu \end{pmatrix} \times \mathrm{Im}Q_{\lambda}(1234),$$

$$Q_{\lambda} = Q_{\lambda}^{\mathrm{Qul}} + Q_{\lambda}^{\mathrm{Br}}, \tag{6}$$

where $j_i$ is the total single electron momentums, $m_i$ – the projections; $Q^{Qul}$ is the Coulomb part of interaction, $Q^{Br}$ - the Breit part. The imaginary part $Q_{\lambda}^{Cul}$ contains the radial $R_{\lambda}$ and angular $S_{\lambda}$ integrals as follows:

$$\begin{aligned}\mathrm{Im}\,Q_{\lambda}^{Cul}(12;43) = Z^{-1}\,\mathrm{Im}\{&R_{\lambda}(12;43)S_{\lambda}(12;43) + R_{\lambda}(\tilde{1}2;4\tilde{3})S_{\lambda}(\tilde{1}2;4\tilde{3}) + \\ &+R_{\lambda}(1\tilde{2};\tilde{4}3)S_{\lambda}(1\tilde{2};\tilde{4}3) + R_{\lambda}(\tilde{1}\tilde{2};\tilde{4}\tilde{3})S_{\lambda}(\tilde{1}\tilde{2};\tilde{4}\tilde{3})\}.\end{aligned} \tag{7}$$

The angular coefficient has only a real part:

$$S_{\lambda}(12;43) = S_{\lambda}(13)S_{\lambda}(24) \qquad S_{\lambda}(13) = \{\lambda l_1 l_3\}\begin{pmatrix} j_1 & j_3 & \lambda \\ \frac{1}{2} & -\frac{1}{2} & 0 \end{pmatrix} \tag{8}$$

$\{\lambda l_1 l_3\}$ means that $\lambda, l_1$ and $l_3$ must satisfy the triangle rule and the sum $\lambda + l_1 + l_3$ must be an even number. The rest terms in (7) include the small components of the Dirac functions. The tilde designates that the large radial component $f$ must be replaced by the small one $g$, and instead of $l_i, \tilde{l}_i = l_i - 1$ should be taken for $j_i < l_i$ and $\tilde{l}_i = l_i + 1$ for $j_i > l_i$. The Breit (magnetic) part can be expressed as follows [27]:

$$Q_{\lambda}^{Br} = Q_{\lambda,\lambda-1}^{Br} + Q_{\lambda,\lambda}^{Br} + Q_{\lambda,\lambda+1}^{Br} \tag{9}$$

The corresponding imaginary part (17) is as follows:

$$\begin{aligned}\mathrm{Im}\,Q_{\lambda,l}^{Br} = \frac{1}{Z}\mathrm{Im}\{&R_{\lambda}(12;\tilde{4}\tilde{3})S_{\lambda}^{l}(12;\tilde{4}\tilde{3}) + R_{\lambda}(\tilde{1}\tilde{2};43)S_{\lambda}^{l}(\tilde{1}\tilde{2};43) + \\ &+R_{\lambda}(\tilde{1}2;\tilde{4}3)S_{\lambda}^{l}(\tilde{1}2;\tilde{4}3) + R_{\lambda}(\tilde{1}\tilde{2};\tilde{4}\tilde{3})S_{\lambda}^{l}(\tilde{1}\tilde{2};\tilde{4}\tilde{3})\}.\end{aligned} \tag{10}$$

The detailed expressions for the Coulomb and Breit parts and the corresponding radial $R_{\lambda}$ and angular $S_{\lambda}$ integrals can be found in Refs. [22-32].The total probability of a $\lambda$ - pole transition is usually represented as a sum of the electric $P_{\lambda}^{E}$ and magnetic $P_{\lambda}^{M}$ parts. The electric (or magnetic) $\lambda$ - pole transition $\gamma \to \delta$ connects two states with parities which by $\lambda$ ( or $\lambda$ +1) units. In our designations

$$\begin{aligned}&P_{\lambda}^{E}(\gamma \to \delta) = 2(2j+1)Q_{\lambda}^{E}(\gamma\delta;\gamma\delta) \qquad Q_{\lambda}^{E} = Q_{\lambda}^{Cul} + Q_{\lambda,\lambda-1}^{Br} + Q_{\lambda,\lambda+1}^{Br} \\ &P_{\lambda}^{M}(\gamma \to \delta) = 2(2j+1)Q_{\lambda}^{M}(\gamma\delta;\gamma\delta) \qquad Q_{\lambda}^{M} = Q_{\lambda,\lambda}^{Br}.\end{aligned} \tag{11}$$

In our work the relativistic wave functions are determined by solution of the Dirac equation with the potential, which includes the Ivanova-Ivanov “outer electron- ionic core” potential [22] and polarization potential [32,38]. The calibration of the single model potential parameter has been

performed on the basis of the special ab initio procedure [37,38] (see also [1,29,30]). In Refs. [29,30] the lowest order multielectron effects, in particular, the gauge dependent radiative contribution Im $\delta E_{ninv}$ for the certain class of the photon propagator calibration has been treated. The value of this contribution allows to estimate an effectiveness of quantitative accounting for the multielectron correlation effects. The minimization of the gauge-non-invariant contribution Im $\delta E_{ninv}$ provides a reasonable criterion in the construction of an optimized one-electron representation in the relativistic many-body perturbation theory. The minimization procedure leads to the system of the integral-differential equation that can be solved using one of the standard numerical codes. In result, this provides the construction of the optimized one-particle representation and improves an effectiveness of the numerical code. As it is known (c.f.[1,27]), an accuracy of computing the transition probabilities can be significantly increased by means of adding a multi-electron polarization exchange-correlation potential into the transition amplitude. The correct relativistic expression for the polarization operator has been presented in Refs. [2,36-40] and used by us in this work. All calculations are performed on the basis of the code Superatom-ISAN (version 93).

## 3. Illustration results and conclusions

Here we present some results of computing the oscillator strengths (reduced dipole matrix elements) for a number of transitions in spectra of the heavy alkali atoms and corresponding ions. As the first illustration, we present below the data for the caesium. In Table 1 there are listed the theoretical reduced dipole matrix elements for a number of transitions, computed within: i) relativistic Hartree-Fock (RHF) method [6], ii) the empirical relativistic model potential method (ERMP) [7], iii) the relativistic single-double (SD) method in which single and double excitations of the Dirac-Hartree-Fock (DHF) wave function are included to all orders of perturbation theory [8] and iv) our data. Let us note that the precise experimental data for the $6p_{1/2,3/2}$-6s transition are as follows: $6p_{1/2}$-6s=4.4890(7)and $6p_{3/2}$-6s=6.3238(7) [9]. The important feature of the approach used is using the optimized one-particle representation and an effective account for the exchange-correlation (including the core polarization) effects (see details in Refs. [1,27,38,50]). An estimate of the gauge-non-invariant contributions (the difference between the oscillator strengths values calculated with using the transition operator in the form of "length" G1 and "velocity" G2) is about 0.3%. The REA results, obtained with using the different photon propagator gauges (Coulomb, Babushkin, Landau) are practically equal.

**Table 1.** Theoretical reduced dipole matrix elements for a number of transitions of Cs (see text)

| Transition | i: RHF | ii: ERMP | iii: SD-DHF | iv: Our data |
|---|---|---|---|---|
| $6p_{1/2}$-6s | | 4.489 | 4.482 4.535 | 4.487(G1) 4.488(G2) |
| $7p_{1/2}$-6s | 0.282 | 0.283 | 0.297 0.279 | 0.282 |
| $8p_{1/2}$-6s | | 0.088 | 0.091 0.081 | 0.086 |
| $6p_{3/2}$-6s | | 6.323 | 6.382 6.304 | 6.320 |
| $7p_{3/2}$-6s | 0.582 | 0.583 | 0.601 0.576 | 0.584 |
| $8p_{3/2}$-6s | | 0.228 | 0.232 0.218 | 0.229 |

In figure 1 we present experimental (squares) and theoretical (the empirical Coulomb approximation data by Feng et al – circles [17]; n<40; our work data – continuous line) lifetimes for the Rydberg states $nS_{1/2}$ in spectrum of Cs.

Note that the theoretical results obtained by Feng et al within the empirical Coulomb approximation (n <40), and our computing data are in a good agreement with experimental data. Resulting in the majority only in recent years (see Ref. [46]) experimental data mainly refer to states with n <40.

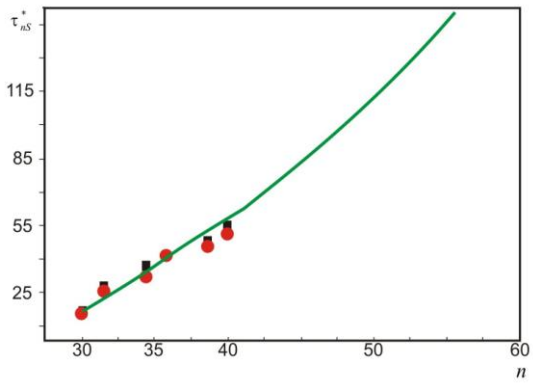


**Figure 1.** Experimental (squares) [17] and theoretical (the empirical Coulomb approximation data by Feng et al – circles; n<40; our work data – continuous line) lifetimes for the Rydberg states $nS_{1/2}$ in spectrum of Cs

Another illustration is computing the transition probabilities in the Ne-like multicharged ions. Let us note that the isoelectronic sequence of neon has been especially thoroughly investigated, but nevertheless remains of interest because of the spectra of Ne-like ions the source of the most important information for the solution of a wide variety of problems in the hot, dense, thermonuclear plasmas spectroscopy, physics of the shortwave lasers etc. The detailed reviews of work on spectroscopy of the Ne-like ions are presented in many papers (look, for example, [27,28,51] and Refs. therein). In tables 2 and 3 we present the values of probabilities of the transitions between levels of the configurations $2s^22p^53s,3d,4s,4d$ and $2s2p^63p,4p$ in the Ne-like ions of the Ni XIX, Br XXVI (in $s^{-1}$; total angle moment J=1): a – the MCDF method; b- relativistic PT with the empirical zeroth approximation (RPTMP); c1 – REA-PT data (without correlation corrections); c2 – REA-PT data (with an account for the correlation); exp.- experimental data (look [17-21,27,28] and Refs therein); This work -our data.

**Table 2.** Probabilities of radiation transitions between levels of the configurations $2s^22p^53s,3d,4s,4d$ and $2s2p^63p,4p$ in the Ne-like ion of Ni XIX (in $s^{-1}$; total angle moment J=1): a – the MCDF method; b- relativistic PT with the empirical zeroth approximation (RPTMP); c1,2 – REA PT data (without and with account for correlation corrections); exp.- experimental data; this work-our data (see text).

| Level *J*=1 | Exp. | a-MCDF | b-RPTMP | c1-REA PT | c2-REA PT | This work |
|---|---|---|---|---|---|---|
| $2p_{3/2}3s_{1/2}$ | 7.6+11 | 9.5+11 | 1.3+12 | 9.7+11 | 8.1+11 | 7.9+11 |
| $2p_{1/2}3s_{1/2}$ | 6.0+11 | 1.8+12 | 1.0+12 | 7.6+11 | 6.2+11 | 6.1+11 |
| $2p_{3/2}3d_{3/2}$ | 1.4+11 | 2.2+11 | 1.5+11 | 1.7+11 | 1.4+11 | 1.3+11 |
| $2p_{3/2}3d_{5/2}$ | 1.2+13 | 2.1+13 | 1.2+13 | 1.5+13 | 1.2+13 | 1.1+13 |
| $2p_{1/2}3d_{3/2}$ | 3.2+13 | 4.8+13 | 3.6+13 | 4.0+13 | 3.3+13 | 3.2+13 |
| $2s_{1/2}\ 3p_{1/2}$ | | | 8.5+11 | 9.5+11 | 8.1+11 | 8.0+11 |
| $2s_{1/2}\ 3p_{3/2}$ | | | 5.1+12 | 5.6+12 | 4.7+12 | 4.6+12 |
| $2p_{3/2}4s_{1/2}$ | 3.3+11 | | 3.6+11 | 4.1+11 | 3.4+11 | 3.3+11 |
| $2p_{1/2}4s_{1/2}$ | 2.0+11 | | 3.0+11 | 3.1+11 | 2.4+11 | 2.2+11 |
| $2p_{3/2}4d_{3/2}$ | 4.5+10 | | 5.2+10 | 5.4+10 | 4.8+10 | 4.6+10 |
| $2p_{3/2}4d_{5/2}$ | 8.3+12 | | 8.3+12 | 9.2+12 | 8.2+12 | 8.1+12 |
| $2p_{1/2}4d_{3/2}$ | 8.1+12 | | 7.9+12 | 8.9+12 | 8.0+12 | 8.0+12 |
| $2s_{1/2}4p_{1/2}$ | | | | 6.3+11 | 5.7+11 | 5.6+11 |
| $2s_{1/2}4p_{3/2}$ | | | | 2.7+12 | 2.4+12 | 2.3+12 |

**Table 3.** Probabilities of radiation transitions between levels of the configurations $2s^2 2p^5 3s,3d,4s,4d$ and $2s2p^6 3p,4p$ in the Ne-like ion of Br XXVI (in $s^{-1}$; total angle moment J=1): a – the DF method; b- RPTMP; c1,2 – REA PT data (without and with account for correlation corrections); exp.- experimental data; this work-our data (see text).

| Level $J$=1 | Exp. | a-MCDF | b-RPTMP | c1-QED PT | c2-QED PT | This work |
|---|---|---|---|---|---|---|
| $2p_{3/2}3s_{1/2}$ | 4.5+12 | 6.2+12 | 4.4+12 | 5.5+12 | 4.4+12 | 4.3+12 |
| $2p_{1/2}3s_{1/2}$ | 3.1+12 | 4.8+12 | 2.8+12 | 3.6+12 | 2.7+12 | 2.6+12 |
| $2p_{3/2}3d_{3/2}$ | 2.8+11 | 3.9+11 | 2.9+11 | 3.5+11 | 2.8+11 | 2.7+11 |
| $2p_{3/2}3d_{5/2}$ | 6.1+13 | 8.0+13 | 6.3+13 | 7.5+13 | 6.1+13 | 6.1+13 |
| $2p_{1/2}3d_{3/2}$ | 8.6+13 | 9.5+13 | 8.7+13 | 9.9+13 | 8.6+13 | 8.5+13 |
| $2s_{1/2}\ 3p_{1/2}$ | 3.9+12 | | 4.2+12 | 4.7+12 | 4.0+12 | 3.9+12 |
| $2s_{1/2}\ 3p_{3/2}$ | 1.4+13 | | 1.5+13 | 1.8+13 | 1.4+13 | 1.3+13 |
| $2p_{3/2}4s_{1/2}$ | 1.1+12 | | 1.2+12 | 1.5+12 | 1.1+12 | 1.1+12 |
| $2p_{1/2}4s_{1/2}$ | 2.1+12 | | 2.5+12 | 2.8+12 | 2.3+12 | 2.2+12 |
| $2p_{3/2}4d_{3/2}$ | 2.8+10 | | 7.3+10 | 6.9+10 | 6.3+10 | 6.0+10 |
| $2p_{3/2}4d_{5/2}$ | | | 2.8+13 | 2.7+13 | 2.3+13 | 2.2+13 |
| $2p_{1/2}4d_{3/2}$ | 2.0+13 | | 2.2+13 | 2.3+13 | 2.0+13 | 1.9+13 |
| $2s_{1/2}4p_{1/2}$ | 2.5+12 | | | 2.9+12 | 2.6+12 | 2.5+12 |
| $2s_{1/2}4p_{3/2}$ | 7.1+12 | | | 8.9+12 | 8.0+12 | 7.8+12 |

Analysis of the data shows that the computational method used provides a physically reasonable agreement between the theoretical and experimental data. Let us note that the transition probabilities values in the different photon propagator gauges are practically equal. Besides, an account of the inter particle (electron) correlation effects is of a great importance.

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