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## DETERMINATION OF RADIATION DECAY PARAMETERS FOR HEAVY COMPLEX ATOMIC SYSTEMS

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**Abstract.** The combined relativistic energy approach and relativistic many-body perturbation theory with the zeroth order ab initio model potential optimized one-particle representation are used for precise computing the energy levels and radiative decay probabilities (radiation amplitudes) of heavy alkali elements, in particular, there are listed data for the $7s_{1/2} - np_{1/2,3/2}$, $np_{1/2,3/2}$-$nd_{3/2,5/2}$ (n=7-10) transitions in Fr and some E1 and E2 transitions in a single ionized $Hg^+$ atom. The comparison of the calculated values with available theoretical and experimental (compillated) data is performed..

**Keywords:** radiative decay parameters, heavy atomic systems, relativistic energy approach

# ВИЗНАЧЕННЯ ПАРАМЕТРІВ РАДІАЦІЙНОГО РОЗПАДУ ДЛЯ ВАЖКИХ СКЛАДНИХ АТОМНИХ СИСТЕМ

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**Анотація.** Комбінований релятивістський енергетичний підхід і релятивістська теорія збурень багатьох тіл з одночасткову оптимізованим потенціалом ab initio моделі нульового порядку використовуються для точного розрахунку рівнів енергії і ймовірностей радіаційного розпаду (радіаційних амплітуд) важких лужних елементів, зокрема, наведені дані для переходів $7s_{1/2} – np_{1/2,3/2}$, $np_{1/2,3/2}$-$nd_{3/2,5/2}$ (n=7-10) в Fr і деяких переходів E1 і E2 в однократно іонізованому атомі Hg. Проведено порівняння розрахункових значень з наявними теоретичними і експериментальними (узагальненими) даними.

**Ключові слова:** параметри радіаційного розпаду, важкі атомні системи, релятивістський енергетичний підхід

# ОПРЕДЕЛЕНИЕ ПАРАМЕТРОВ РАДИАЦИОННОГО РАСПАДА ДЛЯ ТЯЖЕЛЫХ СЛОЖНЫХ АТОМНЫХ СИСТЕМ

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**Аннотация.** Комбинированный релятивистский энергетический подход и релятивистская теория возмущений многих тел с одночастичным оптимизированным потенциалом ab initio модели нулевого порядка используются для расчета уровней энергии и вероятностей радиационного распада (радиационных амплитуд) тяжелых щелочных элементов, в частности, приведены данные для переходов $7s_{1/2} – np_{1/2,3/2}$, $np_{1/2,3/2}$-$nd_{3/2,5/2}$ (n=7-10) в Fr и некоторых переходов E1 и E2 в однократно ионизированном атоме Hg. Проведено сравнение расчетных значений с имеющимися теоретическими и экспериментальными (обобщенными) данными.

**Ключевые слова:** параметры радиационного распада, тяжелые атомные системы, релятивистский энергетический подход

## 1. Introduction

Study of energy and radiative parameters of complex atomic systems, including systems in highly-excited, Rydberg states is of a great interest to create new quantum (atomic) sensor devices, quantum computer systems etc. It is self-understood that the correct data about different radiation, energetic and spectroscopic characteristics of the multielectron atoms and corresponding ions, namely, radiative decay widths, probabilities and oscillator strengths of atomic transitions, excitation and ionization cross-sections are needed in different atomic, molecular physics topics, laser physics and quantum electronics, as well as in astrophysics and laboratory, thermonuclear plasma diagnostics and in fusion research [1-9]. In this light, a special interest attracts studying the energy and radiative characteristics of the heavy complex atomic systems. There have been sufficiently many reports of calculations and compilation of energies and oscillator strengths for these atoms and corresponding ions (see, for example, [4–

23]). 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.

In order to determine the transition probabilities one usually uses usually a standard amplitude approach. Each of theoretical approaches to calculation of transition probabilities contains critical factors (configuration interaction or multiconfiguration treatment, spectroscopic coupling schemes and relativistic corrections, exchange-correlation corrections convergence of probabilities results and of the dipole length and velocity forms, accuracy of transition energies etc) which need to be adequately taken care of to get reliable results.

One of the powerful approached to studying energy and spectral parameters of complex atomic systems is provided by a relativistic energy approach, which allows correctly to calculate the radiative decay characteristics for atoms and ions and new data on the transition probabilities for some interesting atoms and ions. Originally the energy approach to radiative and autoionization processes in multielectron atoms and ions has been developed by Ivanova-Ivanov et al [10-12]. More advanced version of the relativistic energy approach has been further developed in Refs. [13-15]). The energy approach is based on the Gell-Mann and Low S-matrix formalism combined with the relativistic perturbation theory (PT). In relativistic case the Gell-Mann and Low formula expressed an energy shift $\Delta E$ through the electrodynamical scattering matrix including interaction with as the photon vacuum field as a laser field. The first case is corresponding to determination of radiative decay characteristics for atomic systems. Earlier we have applied the corresponding generalized versions of the energy approach to many problems of atomic, nuclear and even molecular spectroscopy, including, cooperative electron-gamma-nuclear "shake-up" processes, electron-muon-beta-gamma-nuclear spectroscopy, spectroscopy of atoms in a laser field etc [21-29]. Different advanced computational generalizations have been considered in Refs. [16-23].

In this paper the combined relativistic energy approach (REA) [10-13] and relativistic perturbation theory (PT) with the zeroth order ab initio one-particle representation [28-31] is used for computing spectral parameters of the heavy complex systems (Fr, $Hg^+$ ). The comparison of the calculated data with available theoretical and experimental data is performed.

**2. The theoretical method**

In the relativistic energy approach (REA) 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:

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

where $\Gamma$ is interpreted as the level width, and the transition probability $P = \Gamma$. 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 [23,26] 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 $\Delta E$ . 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 [11, 28, 29]:

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

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. It is usually 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 (5) one could have summarized all the contributions of the one -quasiparticle diagrams of all orders of the formally exact relativistic PT. However, the necessary experimental quantities are not often available.

An imaginary part of electron energy can be defined in the lowest order of the perturbation theory as [10-12]:

$$\mathrm{Im}\Delta E(B)=-\frac{e^2}{4\pi}\sum_{\substack{\alpha>n>f\\ [\alpha<n\le f]}} V_{\alpha n\alpha n}^{|\omega_{\alpha n}|}, \qquad (3a)$$

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

$$V_{ijkl}^{|\omega|}=\iint dr_1 dr_2 \Psi_i^*(r_1)\Psi_j^*(r_2)\frac{\sin|\omega|r_{12}}{r_{12}}(1-\alpha_1\alpha_2)\Psi_k^*(r_2)\Psi_l^*(r_1) \qquad (3b)$$

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

$$\Gamma_{\alpha_n}=\frac{1}{4\pi}\cdot V_{\alpha_n\alpha_n}^{|\omega_{\alpha_n}|} \qquad (4)$$

Substitution of the expansion for $\sin|\omega|r_{12}/r_{12}$ on spherical harmonics to matrix element of interaction gives as follows [11,13]:

$$V_{1234}^{\omega}=[(j_1)(j_2)(j_3)(j_4)]^{1/2}\sum_{\lambda\mu}(-1)^{\mu}\begin{pmatrix} j_1 j_3 & \lambda\\ m_1-m_3 & \mu\end{pmatrix}\times \mathrm{Im}\,Q_\lambda(1234) \qquad (5)$$

$$Q_\lambda=Q_\lambda^{\mathrm{Qul}}+Q_\lambda^{\mathrm{Br}}, \qquad (6)$$

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:

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

The angular coefficient has only a real part:

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

$\{\lambda l_1 l_3\}$ 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 detailed expressions for the Coulomb and Breit parts and the corresponding radial $R_\lambda$ and angular $S_\lambda$ integrals can be found in Refs. [11].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 these designations

$$P_\lambda^E(\gamma\to\delta)=2(2j+1)Q_\lambda^E(\gamma\delta;\gamma\delta) \qquad Q_\lambda^E=Q_\lambda^{Cul}+Q_{\lambda,\lambda-1}^{Br}+Q_{\lambda,\lambda+1}^{Br}$$
$$P_\lambda^M(\gamma\to\delta)=2(2j+1)Q_\lambda^M(\gamma\delta;\gamma\delta) \qquad Q_\lambda^M=Q_{\lambda,\lambda}^{Br}. \qquad (9)$$

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 [10] and polarization potential [4]. The calibration of the single model potential parameter has been performed on the basis of the special ab initio procedure [13,29]. In Refs. [13] 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. [3,4] and used by us in this work. All calculations are performed on the basis of the code Superatom (version 93).

### 3. The results and conclusions

We applied the above described approach to compute the oscillator strengths (reduced dipole matrix elements) for a number of transitions in spectra of the heavy alkali atom of francium. 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, ii) the empirical relativistic model potential method (ERMP), 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 [5] and iv) our data. Let us note that the precise experimental data for the $7p_{1/2,3/2}$-7s transition are as follows: $7p_{1/2}$-7s=4.277 and $7p_{3/2}$-7s=5.898 [9]. The important features of the approach used are using the optimized one-particle representation and an effective taking into account the exchange-correlation (including the core polarization) effects (see Refs. [3,4,11,38-31]). 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.

Further we present the data of calculations of the energies and probabilities of radiation transitions (oscillator forces), in particular, E1 transitions: $5d^{10}7p(P_{1/2},P_{3/2})$-$5d^{10}6s(S_{1/2})$, $5d^{10}7p(P_{1/2},P_{3/2})$-$5d^{10}7s(S_{1/2})$, E2 quadrupole transition $5d^9 6s^2 (D_{5/2},D_{3/2})$- $5d^{10}6s$ $(S_{1/2})$ in a single ionized $Hg^+$ atom. It should be noted that the ion is characterized by, firstly, not good enough level of study of spectral characteristics, and secondly, it is very interesting from the point of view of necessity of correct consideration of both relativistic and correlation corrections, since the transitions pass in a sufficiently strong field of the nucleus with charge Z = 80 . Within our formalism, the above states are usually interpreted as one- and three-quasiparticle electron states (6s) (vacancies $5d^{-1}$) above the skeleton of filled electron shells $5d^{10}6s^2$.

In Tables 2.3, we provide our theory data as well as experimental data (Moore, NBS) and alternative theoretical calculations of the energies and probabilities of dipole E1 transitions $5d^{10}7p(P_{1/2},P_{3/2})$-$5d^{10}6s(S_{1/2})$, $5d^{10}7p(P_{1/2},P_{3/2})$-$5d^{10}7s(S_{1/2})$, E2 quadrupole transition $5d^9 6s^2 (D_{5/2},D_{3/2})$- $5d^{10}6s$ $(S_{1/2})$ in $Hg^+$ (HF - Hartree-Fock data, DF - Dirac-Fockdata, DF (exp.) – Dirac-Fock (using experimental transition lengths), RPT-MP - data of relativistic PT with model potential (MP) zero approximation, Our-our theory; Exp. – experimental data (from NBS) [4,7,30]. The analysis of the presented data shows that, first, the standard methods HF, DF in a single-configuration variant give a very high error in the calculation of energies and probabilities of radiation transitions, and when used in the DF scheme of experimental transition lengths, the accuracy of calculations is significantly , since it is obvious that using empirical data makes it possible to efficiently take into account some of the very important in quantitative terms of correlation corrections

Table 1

**Theoretical reduced dipole matrix elements for a number of transitions of Fr (see text)**

| Transition | i: RHF | ii: ERMP | iii: SD-DHF | iv: Our data |
|---|---|---|---|---|
| $7p_{1/2}$-7s | 4.279 4.304 | - | 4.256 | 4.272 (G1)<br>4.274 (G2) |
| $8p_{1/2}$-7s | 0.291 0.301 | 0.304 | 0.327 0.306 | 0.339 |
| $9p_{1/2}$-7s | - | 0.096 | 0.110 | 0.092 |
| $7p_{3/2}$-7s | 5.894 5.927 | - | 5.851 | 5.891 |
| $8p_{3/2}$-7s | 0.924 | 0.908 | 0.934 0.909 | 0.918 |
| $9p_{3/2}$-7s | - | 0.420 | 0.436 | 0.426 |

Table 2.

**Transitions energies for $5d^{10}7p(P_{1/2},P_{3/2})$-$5d^{10}6s(S_{1/2})$, $5d^{10}7p(P_{1/2},P_{3/2})$-$5d^{10}7s(S_{1/2})$, $5d^{9}6s^{2}(D_{5/2},D_{3/2})$-$5d^{10}6s$ $(S_{1/2})$ in $Hg^{+}$ (in Ry): HF - Hartree-Fock data, DF - Dirac-Fockdata, DF (exp.) – Dirac-Fock (using experimental transition lengths), RPT-MP - data of relativistic PT with model potential (MP) zero approximation, Our-our theory; Exp. – experimental data (from NBS);**

| Method | $E_{6s}$ | $7P_{1/2}$-$6S_{1/2}$ | $7P_{3/2}$-$6S_{1/2}$ | $7P_{1/2}$- $7S_{1/2}$ | $7P_{3/2}$-$7S_{1/2}$ | $D_{3/2}$- $S_{1/2}$ | $D_{5/2}$- $S_{1/2}$ |
|---|---|---|---|---|---|---|---|
| Exp. | -1.378 | 0.987 | 1.020 | 0.115 | 0.148 | 0.461 | 0.324 |
| HF | -1.07 | 0.721 | 0.721 | 0.095 | 0.095 | 0.863 | 0.863 |
| DF | -1.277 | 0.904 | 0.922 | 0.109 | 0.127 | 0.608 | 0.460 |
| RPT-MP | -1.377 | 0.986 | 1.019 | 0.114 | 0.147 | 0.462 | 0.325 |
| Our | -1.378 | 0.987 | 1.020 | 0.115 | 0.148 | 0.462 | 0.324 |

Table 3.

**Probabilities of E1 transitions $5d^{10}7p(P_{1/2},P_{3/2})$-$5d^{10}6s(S_{1/2})$, $5d^{10}7p(P_{1/2},P_{3/2})$-$5d^{10}7s(S_{1/2})$ in Hg + (in $s^{-1}$): HF - Hartree-Fock data, DF - Dirac-Fockdata, DF (exp.) – Dirac-Fock (using experimental transition lengths), RPT-MP - data of relativistic PT with model potential (MP) zero approximation, Our-our theory; Exp. – experimental data (from NBS);**

| Method | $7P_{3/2}$-$6S_{1/2}$ | $7P_{1/2}$- $6S_{1/2}$ | $7P_{3/2}$- $7S_{1/2}$ | $7P_{1/2}$- $7S_{1/2}$ | $D_{3/2}$- $S_{1/2}$* | $D_{5/2}$- $S_{1/2}$* |
|---|---|---|---|---|---|---|
| Exp. | $1.53\cdot10^{8}$ | $2.35\cdot10^{7}$ | $1.44\cdot10^{8}$ | $6.37\cdot10^{7}$ | 53.5±2.0 | 11.6±0.4 |
| HF | $4.75\cdot10^{6}$ | $4.75\cdot10^{6}$ | $3.65\cdot10^{7}$ | $3.65\cdot10^{7}$ | 1360 | 1360 |
| DF | $8.45\cdot10^{7}$ | $1.67\cdot10^{7}$ | $6.89\cdot10^{7}$ | $4.71\cdot10^{7}$ | 257.0 | 77.4 |
| DF ($E_{exp}$) | $1.17\cdot10^{8}$ | $2.04\cdot10^{7}$ | $1.10\cdot10^{8}$ | $5.52\cdot10^{7}$ | 63.9 | 13.3 |
| RPT-MP | $1.49\cdot10^{8}$ | $2.31\cdot10^{7}$ | $1.41\cdot10^{8}$ | $6.33\cdot10^{7}$ | 54.53 | 11.84 |
| Our | $1.51\cdot10^{8}$ | $2.33\cdot10^{7}$ | $1.43\cdot10^{8}$ | $6.35\cdot10^{7}$ | 53.84 | 11.72 |

Note: *$5d^{9}6s^{2}(D_{5/2},D_{3/2})$- $5d^{10}6s$ $(S_{1/2})$;

Our theory consistently performs an efficient accurate account of the main exchange-correlation effects, which will include the effects of the mutual shielding of particles, the exchange-polarization quasiparticles through the polarizable many-electron core, as well as their interaction with the atomic core through photonic vacuum, iterative corrections and other. This, as a result, provides a physically reasonable agreement between theory and experiment.

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# DETERMINATION OF RADIATION DECAY PARAMETERS FOR HEAVY COMPLEX ATOMIC SYSTEMS

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## Summary

Study of energy and radiative parameters of complex atomic systems, including systems in highly-excited, Rydberg states is of a great interest to create new quantum (atomic) sensor devices, quantum computer systems as well as for different atomic and laser physics and quantum electronics. The combined relativistic energy approach and relativistic many-body perturbation theory with the zeroth order ab initio model potential optimized one-particle representation are used for precise computing the energy levels and radiative decay probabilities (radiation amplitudes) of heavy alkali elements (francium) and singly ionized atom of Hg. There are listed data for the $7s_{1/2} - np_{1/2,3/2}$, $np_{1/2,3/2}$-$nd_{3/2,5/2}$ (n=7-10) transitions in Fr and the energies and probabilities of radiation transitions (oscillator forces), in particular, E1 transitions: $5d^{10}7p(P_{1/2},P_{3/2})$-$5d^{10}6s(S_{1/2})$, $5d^{10}7p(P_{1/2},P_{3/2})$-$5d^{10}7s(S_{1/2})$, E2 quadrupole transition $5d^9 6s^2 (D_{5/2},D_{3/2})$- $5d^{10}6s (S_{1/2})$ in a single ionized $Hg^+$ atom. The comparison of the calculated values with available theoretical and experimental (compillated) data is performed. The analysis of the presented data shows that, first, the standard methods HF, DF in a single-configuration variant give a very high error in the calculation of energies and probabilities of radiation transitions, and when used in the DF scheme of experimental transition lengths, the accuracy of calculations is significantly , since it is obvious that using empirical data makes it possible to efficiently take into account some of the very important in quantitative terms of correlation corrections. Our theory consistently performs an efficient accurate account of the main exchange-correlation effects, which will include the effects of the mutual shielding of particles, the exchange-polarization quasiparticles interaction through the polarizable many-electron core and others.

**Keywords:** radiative decay parameters, heavy atomic systems, relativistic energy approach

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# ВИЗНАЧЕННЯ ПАРАМЕТРІВ РАДІАЦІЙНОГО РОЗПАДУ ДЛЯ ВАЖКИХ СКЛАДНИХ АТОМНИХ СИСТЕМ

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## Реферат

Вивчення енергетичних та випромінювальних параметрів складних атомних систем, включаючи системи у високо збуджених та рідбергівських станах, представляє великий інтерес для створення нових квантових (атомних) сенсорних пристроїв, квантових комп'ютерних систем, а також для різних задач атомної і лазерної фізики та квантової електроніки. Комбінований релятивістський енергетичний підхід і релятивістська багаточастинкова теорія збурень з оптимізованим модельним наближенням використовуються для точного розрахунку рівнів енергії і ймовірностей радіаційного розпаду (радіаційних амплітуд) важких лужних елементів (францій) і одноіонізованого атома Hg. Перераховані дані для переходів $7s_{1/2} - np_{1/2,3/2}$, $np_{1/2,3/2}$-$nd_{3/2,5/2}$ (n=7-10) у Fr та енергій та ймовірностей випромінювання переходи (коливальні сили), зокрема, переходи E1: $5d^{10}7p(P_{1/2},P_{3/2})$-$5d^{10}6s(S_{1/2})$, $5d^{10}7p(P_{1/2},P_{3/2})$-$5d^{10}7s(S_{1/2})$, E2 перехід $5d^9\,6s^2\,(D_{5/2},D_{3/2})$- $5d^{10}6s\,(S_{1/2})$ в однократно у іонізованому атомі Hg. Проводиться порівняння обчислених значень з наявними теоретичними та експериментальними (складеними) даними. Аналіз представлених даних показує, що, по-перше, стандартні методи тпу Хартрі-Фока та Дірака-Фока (ДФ) в одноконфігураційному варіанті дають дуже високу похибку в обчисленні енергій і ймовірностей радіаційних переходів і при використанні в схемі ДФ експериментальних довжин переходу точність обчислень суттєво зростає, оскільки використання емпіричних даних дозволяє ефективно врахувати деякі дуже важливі в кількісному відношенні кореляційні поправки. Розвинута теорія послідовно виконує ефективне урахування основних обмінно-кореляційних ефектів, зокрема, ефектів взаємного екранування частинок, обмінно-поляризаційну взаємодію квазічастинок через поляризує мий багатоелектронний остов та інші.

**Ключові слова:** параметри радіаційного розпаду, важкі атомні системи, релятивістський енергетичний підхід