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A.V. Glushkov, O.Y. Khetselius, A.A. Svinarenko

MATHEMATICAL PHYSICS OF CLASSICAL AND QUANTUM SYSTEMS. Part 2

Textbook

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In the textbook "Mathematical Physics of Classical and Quantum Systems", part 2, the basic issues of modern mathematical physics of quantum systems, elements of quantum geometry, algebra, mechanics, electrodynamics in the aspects of determining energy parameters of quantum systems and calculation of dynamic, energy and spectral characteristics of energy levels of atoms are described and ions, etc.

It can be used by PhD students (magisters (partly) and scientific workers) of the specialities: 113-"Applied Mathematics", and 111-"Mathematics", 104- "Physics and Astronomy", and so on.

Reviewers:
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INTRODUCTION

The discipline "Mathematical Physics of Classical and Quantum Systems. Quantum" is an important discipline in the cycle of professional training of postgraduate students (third level of education) in specialty 113- Applied Mathematics.

It is aimed at assimilating (assuring) a number of planned competencies, including the study of a modern apparatus of quantum geometry and dynamics of resonances, as well as new applied (computational) methods and algorithms for calculating the fundamental energy (radiation) characteristics of resonances (resonance states) of complex classical and quantum systems with possible generalizations on various classes of mathematical, physico-chemical, cybernetic, socio-economic and ecological systems, use of modern scientific m todiv scientific results and achievements that create potentially new knowledge in the field of quantum geometry and dynamics rezonsniv.

The place of discipline in the structural-logical scheme of its teaching: the knowledge obtained in the study of this discipline is used in writing dissertation papers, the topics of which are related to the study of fundamental energy (radiation) characteristics of resonances (resonance states) of complex classical and quantum systems with possible generalizations on a variety classes of mathematical, physico-chemical, cybernetic, socio-economic and ecological systems.

The basic concepts of discipline are the desirable tools of an experienced specialist in the field of applied mathematics.

The purpose of studying discipline is assimilation (assurance) of a number of competencies, in particular, mastering the modern apparatus of quantum geometry and resonance dynamics, the ability to develop new and improve existing mathematical methods for analysis, modeling and prediction of energy (radiation) characteristics of resonances (resonance states) of complex classical and quantum systems . After mastering this discipline, the postgraduate student must be able to use modern or develop new approaches, in particular, based on quantum geometry and resonance dynamics, to analyze, simulate, predict, and program the characteristics of resonances (resonance states) of complex classical and quantum systems with the formulation of computer experiments.

It should be noted that the manual widely used new scientific and methodological results in the field of quantum geometry and dynamics of

resonances, in the vast majority of which are obtained directly by the authors of the manual (for example, a description of the relativistic energy approach to the description of autoionization and multiphoton resonances in the spectra of quantum systems, for example, in the microwave field, etc.), as well as in the author's wording, the fundamental fundamental questions, as well as the most significant scientific results in the field of quantum geometry and dynamics ing resonances obtained international team of leading academic experts. Some sections of the textbook contain, as indicated, fundamentally new scientific results.

Among them, particular attention should be paid to the following:

1). Theoretical bases of the new, precision relativistic method of description and calculation of characteristics of multiphoton processes for atoms in the field of intensive laser radiation on the basis of CED theory of perturbations, the method of relativistic Green's functions,

2) for the first time in the world based on its quantitative modeling of energy and radiation properties of multiphoton resonances in spectra of a number of complex atoms, and others.

In addition, most of the most significant new results and developments have been tested and presented at a number of leading professional conferences, schools, congresses, including the VI-XXIV International Workshop on Quantum Systems in Chemistry and Physics (VI-Upssala, Sveden; XXIII-SouthAfrica;, 47th Conference of the European Group Atomic Systems (EGAS-47, Riga, Latvia, 2015), XXIX International Conference on Photonic, Electronic, and Atomic Collisions (ICPEAC, Toledo, Spain, 2015), III, IV, V International School and Conference on Photonics (Belgrade, Serbia, 2013-2015), 21st Central European Workshop on Quantum Optics (Brussels, Belgium, 2014), 22nd International Conference on Spectral Lina Shapes (UT Space Institute, Tullahoma, USA, 2014), 13th International Conference on Artificial Intelligence, Knowledge Engineering and Data Bases (Gdansk, Poland, 201 4th edition of the 32nd European Congress on Molecular Spectroscopy (Heinrich-Heine-University, Düsseldorf, Germany, 2014), 12th International Conference "Dynamical Systems-Theory and Applications" (Lodz, Poland, 2013), XVIII International Workshop on Quantum Systems in Chemistry and Physics (Paraty-Rio de Janeiro, Brazil, 2013), XI International Conference on Atomic and Molecular Pulsed Lasers (Tomsk, Russia, 2013), 22nd International Laser Physics Workshop (Prague, Czech Republic, 2013),

11th International Colloquium on Atomic Spectra and Oscillator Strengths for Astrophysical and Laboratory Plasmas (Mons, Belgium, 2013), 2nd Chaotic Modeling and Simulation International Conference (Crete, Greece, 2009), International Conference on Statistical Physics (Crete, Greece, 2008) and many others.

Taking this opportunity, the authors express their gratitude to the staff of the Department of Higher and Applied Mathematics of the ODEKU, at scientific and methodological workshops which were devoted to many of the issues outlined in the book, as well as Ph.D., associate professor Buyadzhi V.V., Ph.D., associate professor Ternovsky V.B. as well as well-known leading foreign experts: Prof. E. Brandas (Uppsala, Sweden), Prof. J. Maruani (Paris, France), Prof. S.Wilson (Oxford, The UK) for helpful discussions on a number of questions and advice on setting out some issues of resonance dynamics.

List of abbreviations,constants, units used

MPR – multiphoton resonance (resonances)
DE – differential equation (method)
QED – quantum electrodynamic
LR – laser radiation
REF – relativistic energy formalism
RHF – relativistic approximation Hartree-Fok
PT – perturbation theory
PTDF – many-particle PT with DF zero approximation;
GF – Green's function (method)
AC – alternating current
DF – Dirac-Fock (method)
DKS – Dirac-Kohn-Sham (method)
DC – direct current
LE – Lyapunov's exponents
QP – quasi-particle
XC (effects) – exchange-correlation (effects)
WKB – WKB approximation

Fundamental constants:

Speed of light c=2,997925·10^{8} м/с; Elementary charge e=1,60219·10^{-19} Кл;
Electron mass m=9,1095·10^{-31} кг; Planck constant $\hbar$=1,05459·10^{-34}Дж·с;
Rydberg constant R_{∞}=1,0973732·10^{7}м$^{-1}$ Bore radius $\hbar^2/me^2$=0,5291773 Å;
Fine-structure constant $\alpha=e^2/\hbar c, 1/\alpha$=137,03597;

Units. Everywhere where otherwise indicated, atomic units are used: e=1, $\hbar$=1, m=1 (c=137,03597). Atomic units of length, time and velocity: $\hbar^2/me^2$=5,291773·10^{-11} m, $\hbar^3/me^4$=2,4189·10^{-17} s, $e^2/\hbar$=2,1877·10^{6} m/s. Atomic unit of energy (a.u.e.) $me^4/\hbar^2$=2Ry=27,2116eV=4,3598·10^{-18}J=2,19475·10^{5}cm^{-1} ($me^4/2\hbar^2$= Ry – Rydberg). Energy in Coulomb unts (c.u.): 1 c.u.e.=Z^2 a.u.e. (Z – charge of atomic nucleus). Relativistic units: $\hbar$=1, c=1, m=1, e^2=1/137,03597.

CHAPTER 1. RELATIVISTIC ENERGY APPROACH IN MATHEMATICAL PHYSICS OF TO RADIATIVE AND AUTOIONIZATION PROCESSES IN HEAVY FINITE FERMI-SYSTEMS

1.1 The relativistic Dirac equation for an electron in an external field

As is well known from QED (c.f. Classical Course of theoretical physics [1,2], we follow below) and quantum geometry (see. Eg., [3,4]), the wave equations of free particles express the properties that, In fact, the general requirements associated with the spatio-temporal symmetry.

Naturally occurring particles is dependent on the physical properties of the processes of their interactions. Consistent description of electromagnetic interactions is given by one of the most reasonable physical theories - QED. Of course, it should be recalled that this formalism is used to describe the electromagnetic interactions of a particle is not capable of strong interactions. These particles, of course, are the electrons (and positrons), and thus, for the existing theory is available to the whole vast area electron QED.

The traditional range of tasks in quantum geometry and the theory of QED confined to a single particle. This is - the problem in which the number of particles does not change, and the interaction can be entered using the concept of an external electromagnetic field. In addition to the conditions that enable the external field is considered as a given, the limits of applicability of this theory are also limited conditions associated with so-called QED radiative corrections.

Below in this subchapter the relativistic units $\hbar$=1, c=1, m=1, are used; the square of the electron charge e^2 is replaced by the dimensionless α ($1/\alpha$==137,03597).

One could consider, following [1], the wave equation of the electron in a given external field. As usual, let

$$A^{\mu} = (\Phi, \mathrm{A})$$

- 4-potential of the external electromagnetic field (A- vector, Φ- scalar potentials). Required equation follows from the Dirac equation by replacing the 4-momentum operator difference *p-eA* (*e* – particle charge):

$$\left[\gamma\left(p-eA\right)-m\right]\psi=0\,. \qquad \text{(i1.1)}$$

Here and below we use commonly used in relativistic QED units (see. below). where e^2 is replaced by α.

Corresponding to the Hamiltonian equation can also be obtained by replacing the standard Dirac Hamiltonian:

$$H=\alpha(p-eA)+\beta m+e\Phi\,. \qquad \text{(i1.2)}$$

Naturally, this does not concern the form of radial wavefunctions. In connection with the above, the wave function of the stationary states (in the standard representation) must be sought in the form of:

$$\psi=\begin{pmatrix}\varphi\\ \chi\end{pmatrix}=\begin{pmatrix} f\left(r\right)\Omega_{jlm}\\ \left(-1\right)^{\frac{1+l-l'}{2}}\ g\left(r\right)\Omega_{jl'm}\end{pmatrix}, \qquad \text{(i1.3)}$$

where

$$l=j\pm1/2\,,\ l'=2j-l\,,$$

and the exponent of -1 is introduced to simplify the subsequent formulas.

In classical electrodynamics the electromagnetic interaction is described by the well-known expression:

$$-ej^{\mu}A_{\mu} \qquad \text{(i1.4a)}$$

density langranzhiana "field + charges" (A - 4-potential field j - 4-vector current density of the particles). The current density satisfies the continuity equation:

$$\partial_\mu j^\mu = 0\,,$$

(i1.4b)

expresses the law of conservation of charge.

The electromagnetic interaction operator (the integral over the space of the interaction Hamiltonian density) has the standard form:

$$V_{\text{int}} = e\int \left(\hat{j}A\right) d^3x\,. \qquad \text{(i1.5)}$$

The probability of transition in the quantum system under the influence of the perturbation V_{int} in the first approximation is given by the formula known PT ("golden" rule by Fermi).

It is usually assumed that the initial and final states of the radiating system belong to the discrete spectrum. Then the probability (per unit time) of the transition $i \to f$ with the emission of a photon is given by the well-known formula:

$$d\omega = 2\pi \left|V_{fi}\right|^2 \delta\left(E_i - E_f - \omega\right) d\nu\,, \qquad \text{(i1.6)}$$

where ν conventionally denotes the set of variables that characterize the state of the photon and runs through a continuous range of values (in this case the photon wave function is assumed normalized to δ-function "scale ν").

If the photon is emitted with a certain value of the moment, the only variable is the continuous frequency ω. Integration of the formula (1.6) to $d\nu \equiv d\omega$ eliminate δ-function (replacing ω the value $\omega = E_i - E_f$), and then the transition probability is determined simply by the expression:

$$\omega = 2\pi \left|V_{fi}\right|^2\,. \qquad \text{(i1.7)}$$

It is assumed that the photon wave function (plane wave) is normalized to one photon in the volume $V = 1$ and $d\nu$ - the number of states have accounted for the phase volume Vd^3k.

As a result, the probability of emission of a photon with a given momentum can obtain the following well-known expression:

$$d\omega = 2\pi \left|V_{fi}\right|^2 \delta\left(E_i - E_f - \omega\right) \frac{d^3k}{\left(2\pi\right)^3}, \qquad \text{(i1.8)}$$

or after integration by $d\omega$:

$$d\omega = \frac{1}{4\pi^2} \left|V_{fi}\right|^2 \omega^2 do\,. \qquad (1.9)$$

As V_{fi} in (i1.8) is substituted matrix element of the form:

$$V_{fi} = e\sqrt{4\pi}\, \frac{1}{\sqrt{2\omega}}\, e^*_\mu j^\mu_{fi}\left(k\right). \qquad \text{(i1.10)}$$

Further, it is useful to remind the formulas relating to dipole radiation. Recall E1 radiative transitions are the most intense in the atomic spectra, and M1 - respectively in nuclear systems. Transition current in this case is the matrix element of the operator

$$\hat{j} = \overline{\psi}\gamma\psi\,,$$

in which the ψ-operators are assumed to expansions in the wave functions of the stationary states of the electron in this field.

Substitution V_{fi} gives the well-known expression for the probability of radiation into the solid angle do of a photon with polarization e:

$$d\omega_{en} = e^2\, \frac{\omega}{2\pi} \left|\mathrm{e}^* \mathrm{j}_{fi}\left(\mathrm{k}\right)\right|^2 do\,, \qquad \text{(i1.11)}$$

where

$$\mathrm{j}_{fi}\left(\mathrm{k}\right) = \int \psi^*_f \alpha \psi_i e^{-i\mathrm{kr}} d^3x\,. \qquad \text{(i1.12)}$$

Here the summation over photon polarizations is done by averaging over the directions of **e** (in a plane perpendicular to a given direction $\mathrm{n} = \mathrm{k}/\omega$) and then the result is multiplied by 2, respectively, to two independent features transverse photon polarization.

As a result, the final expression takes the form:

$$d\omega_n = e^2 \frac{\omega}{2\pi} \left| \left[\mathrm{n} \mathrm{j}_{fi}(\mathrm{k}) \right] \right|^2 do . \qquad \text{(i1.13)}$$

It is appropriate to recall that, as a rule, first consider the case where the photon wavelength λ large compared with the size of the radiating system *a* and that is usually associated with the smallness of the particle velocities compared to the speed of light. In the first approximation in a/λ (corresponding to dipole radiation) in the current transition (i1.12) factor $e^{-i\mathrm{kr}}$ (varies little in the area where ψ_i or ψ_f significantly different from zero) for obvious reasons, is replaced by 1. In fact, the change means neglecting photon momentum compared with the momenta of the particles in the system . Further, the integral $\mathrm{j}_{fi}(0)$ can be replaced by its non-relativistic expression, ie, a matrix element v_{fi} of the electron velocity with respect to the Schrödinger wave functions. Seeking matrix element can be expressed as:

$$v_{fi} = -i\omega \mathrm{r}_{fi} , \qquad (1.14)$$

and

$$e\mathrm{r}_{fi} = \mathrm{d}_{fi} , \qquad \text{(i1.15)}$$

where **d** - the dipole moment of the electron (in its orbital motion).

As a result, we can come to the following classical formula for the probability of dipole radiation:

$$d\omega_{en} = \frac{\omega^3}{2\pi} \left| \mathrm{e}^* \mathrm{d}_{fi} \right|^2 do \qquad \text{(i1.16)}$$

(and direction **n** appears here in an implicit form: vector **e** must be perpendicular to **n**). Summation over polarizations gives:

$$d\omega_n = \frac{\omega^3}{2\pi}\left|\left[\mathrm{n}\,\mathrm{d}_{fi}\right]\right|^2 do. \qquad \text{(i1.17)}$$

Under d_{fi} here obviously refers to a matrix element of the dipole moment of the complete system.

Integration of the formula (1.17) in all directions allows to obtain the following well-known expression for the total probability of radiation:

$$\omega = \frac{4\omega^3}{3}\left|\mathrm{d}_{fi}\right|^2, \qquad \text{(i1.18)}$$

In conventional terms, this formula has the form:

$$\omega = \frac{4\omega^3}{3\hbar c^3}\left|\mathrm{d}_{fi}\right|^2. \qquad \text{(i1.19)}$$

Recall that the radiation intensity I is obtained by multiplying the probability for $\hbar\omega$ that is

$$I = \frac{4\omega^4}{3c^3}\left|\mathrm{d}_{fi}\right|^2. \qquad \text{(i1.20)}$$

Next, consider the elements of the theory of electric and magnetic multipole radiation.

In the light of the material presented above, it is convenient to restrict in this section considering the emission of a photon with definite values of the angular momentum j and its projection m on a chosen direction.

As is known, such photons can be of two types - electric and magnetic. Consider the electric multipole radiation.

We assume that the size of the radiating system are small compared with the wavelength. Following [1-3], it is possible to perform all the calculations using the photon wave functions in the momentum representation, ie, presenting a 4-vector $A^{\mu}(\mathrm{r})$ in the form of a Fourier integral.

The transition matrix element:

$$V_{fi} = e\int j^{\mu}_{ji}(\mathrm{r})\,A^{*}_{\mu}(\mathrm{r})d^3x = e\int d^3x\cdot j^{\mu}_{fi}(\mathrm{r})\int \frac{d^3k}{(2\pi)^3}A^{*}(\mathrm{r})e^{-ikr} \qquad \text{(i1.21)}$$

In order to simplify the notation is convenient to omit the indices ωjm of the photon wave functions. Next to Ej-photon use wave function (2.vector potential):

$$\vec{A}^{э}_{\omega jm}(\vec{k}) = \frac{4\pi^2}{\omega^{3/2}}\delta(|\vec{k}|-\omega)(\vec{Y}^{э}_{jm} + C\vec{n}Y_{jm}) \qquad \text{(i1.22)}$$

$$\Phi^{(э)}_{\omega jm}(\vec{k}) = \frac{4\pi^2}{\omega^{3/2}}\delta(|\vec{k}|-\omega)CY_{jm}$$

with an arbitrary gauge constant C equal to, say,

$$C = -\sqrt{\frac{j+1}{j}}\,.$$

With this choice in the spatial components of the wave function (A) is reduced members comprising spherical harmonics of order $j-1$ and, accordingly, $\vec{A}^{э}_{\omega jm}$ comprises only the order of spherical harmonics $j+1$, resulting in the corresponding contribution V_{fi} is higher order (in a/λ) than the contribution from the components $A^0 \equiv \Phi$, containing spherical functions of lower order j. That is, it should be:

$$A^{\mu} = (\Phi, 0),$$

$$\Phi = -\sqrt{\frac{j+1}{j}} \frac{4\pi^2}{\omega^{3/2}} \delta(|\mathrm{k}| - \omega) Y_{jm}(\mathrm{n})$$

(is there $\mathrm{n} = \mathrm{k}/\omega$). Substituting this expression into (i1.21) and integrating with respect to $|\mathrm{k}|$, please contact:

$$V_{fi} = -e\sqrt{\frac{j+1}{j}} \frac{\sqrt{\omega}}{2\pi} \int d^3x \cdot \rho_{fi}(\mathrm{r}) \int do_{\mathrm{n}} e^{-ikr} Y^*_{jm}(\mathrm{n}). \qquad \text{(i1.23)}$$

Usually to calculate the inner integral is used decomposition:

$$e^{ikr} = 4\pi \sum_{l=0}^{\infty} \sum_{m=-l}^{l} i^l g_l(kr) Y^*_{lm}\left(\frac{\mathrm{k}}{r}\right) Y_{lm}\left(\frac{\mathrm{r}}{r}\right), \qquad \text{(i1.24a)}$$

where

$$g_l(kr) = \sqrt{\frac{\pi}{2kr}} J_{l+1/2}(kr). \qquad \text{(i1.24b)}$$

The final expression for the matrix element of the transition is as follows:

$$V_{fi} = (-1)^{m+1} i^j \sqrt{\frac{(2j+1)(j+1)}{\pi j}} \frac{\omega^{j+1/2}}{(2j+1)!!} e\left(Q^{(э)}_{j,-m}\right)_{fi}. \qquad \text{(i1.25)}$$

Here we have introduced the value of $Q^{(2.e)}$, which are commonly referred to as 2^j-dipole electric moments of transition of the system, by analogy with corresponding classical values:

$$\left(Q^{(э)}_{jm}\right)_{fi} = \sqrt{\frac{4\pi}{2j+1}} \int \rho_{fi}(\mathrm{r}) r^j Y_{jm}\left(\frac{\mathrm{r}}{r}\right) d^3x \qquad \text{(i1.26)}$$

Next, consider the magnetic multipole radiation. The photon wave function of the magnetic type $A^{\mu} = (0, \vec{A})$, where $\vec{A}$ is given by:

$$\vec{A}_{\omega jm}(\vec{k}) = \frac{4\pi^2}{\omega^{3/2}} \delta(|\vec{k}| - \omega) \vec{Y}_{jm}(\vec{n}). \qquad \text{(i1.27)}$$

Using (1.27), one could obtain for the transition matrix element expression:

$$V_{fi} = -e \frac{\sqrt{\omega}}{2\pi} \int d^3x \cdot \mathrm{j}_{fi}(\mathrm{r}) \int do_{\mathrm{n}} \cdot e^{-i\mathrm{kr}} \mathrm{Y}_{jm}^{(м)*}(\mathrm{n}). \qquad \text{(i1.28a)}$$

Vector components $\mathrm{Y}_{jm}^{(м)}$ are expressed in terms of spherical functions of order *j* known formulas (given in [1]).

Further, as above, using the expansion of (1.43) is appropriate and the formula:

$$\int e^{-i\mathrm{kr}} \mathrm{Y}_{jm}^{(м)*}(\mathrm{n}) do_{\mathrm{n}} = 4\pi i^{-j} g_j(kr) \mathrm{Y}_{jm}^{(м)*}\left(\frac{\mathrm{r}}{r}\right),$$

and after substitution g_j:

$$V_{fi} = -ei^{-j} \frac{2\omega^{j+\frac{1}{2}}}{(2j+1)!!} \int \mathrm{j}_{fi}(\mathrm{r}) r^j \mathrm{Y}_{jm}^{(м)*}\left(\frac{\mathrm{r}}{r}\right) d^3x .$$

It is necessary to substitute the function definition $\mathrm{Y}_{jm}^{(м)}$:

$$\mathrm{Y}_{jm}^{(м)}\left(\frac{\mathrm{r}}{r}\right) = \frac{1}{\sqrt{j(j+1)}} \left[\mathrm{r} \nabla Y_{jm}\right].$$

After that the transformation of the integral:

$$\mathrm{r}^{j}\,\mathrm{j}_{fi}\left[\mathrm{r}\nabla Y^{*}_{jm}\right]=-\left[\mathrm{r}\,\mathrm{j}_{fi}\right]\nabla\left[r^{j}Y^{*}_{jm}\right]$$

and finally obtained as a result of the "classical" form [1]:

$$V_{fi}=(-1)^{m}\,i^{j}\sqrt{\frac{(2j+1)(j+1)}{\pi j}}\,\frac{\omega^{j+\frac{1}{2}}}{(2j+1)!!}\,e\left(Q^{(\mathcal{M})}_{j,-m}\right)_{fi},$$

(i1.28b)

where we have introduced 2^{j} -dipole magnetic moments of transition:

$$\left(Q^{(\mathcal{M})}_{jm}\right)_{fi}=\frac{1}{j+1}\sqrt{\frac{4\pi}{2j+1}}\int\left[\mathrm{r}\,\mathrm{j}_{fi}\right]\nabla\left(r^{j}Y_{jm}\right)d^{3}x\,.$$

(i1.29)

As between the expressions (1.29) and (1.26) there is an obvious analogy, in this case, the probability of emission, the formula differs from (1.26) only in the replacement of electric magnetic moments.

The total probability of $M1$-radiation expressed in terms of this value by the standard formula (in conventional units):

$$\omega=\frac{4\omega^{3}}{3\hbar\mathrm{c}^{3}}\left|\mu_{fi}\right|^{2}.$$

(i1.30)

where all constants are the standard.

1.2 QED perturbation theory method for calculation of heavy atoms and multicharged ions

We present the generalized energy approach (Gell-Mann and Low S-matrix formalism) to relativistic calculation of the radiative and autoionization characteristics for multielectron atoms and ions. The approach is based on the Gell-

Mann and Low S-matrix formalism and the gauge-invariant QED perturbation theory (PT) with using the optimized one-quasiparticle representation and an accurate account of the relativistic, correlation and other effects. In relativistic case the Gell-Mann and Low formula expresses an energy shift ΔE through the QED scattering matrix including the interaction with as the laser field as the photon vacuum field. The last case is corresponding to definition of the traditional radiative characteristics for atoms and ions.

Traditionally an investigation of spectra, spectral, radiative and autoionization characteristics for heavy and superheavy elements atoms and multicharged ions is of a great interest for further development atomic and nuclear theories and different applications in the plasma chemistry, astrophysics, laser physics, etc. (see Refs. [1–160]). Theoretical methods of calculation of the spectroscopic characteristics for heavy atoms and ions may be divided into a few main groups. First, the well known, classical multi-configuration Hartree-Fock method (as a rule, the relativistic effects are taken into account in the Pauli approximation or Breit hamiltonian etc.) allowed to get a great number of the useful spectral information about light and not heavy atomic systems, but in fact it provides only qualitative description of spectra of the heavy and superheavy ions (see Refs. [34-36]). superheavy ions. Second, the multi-configuration Dirac-Fock (MCDF) method (see Refs. [1–12, 40-71]) is the most reliable version of calculation for multielectron systems with a large nuclear charge. In these calculations the one- and two-particle relativistic effects are taken into account practically precisely. The calculation program of Desclaux (the Desclaux program, Dirac package) is compiled with proper account of the finiteness of the nucleus size. However, a detailed description of the role of the different nuclear effects (finite nuclear size etc.) is lacking. Though, in last years there is a great progress in this topic. Naturally, the well known relativistic density functional Dirac-Kohn-Sham approach [29,30] (see also Refs. [3,4,31-33,119]) should be mentioned.

In a region of the small Z (Z is a charge of the nucleus) the calculation error in the MCDF approximation is connected mainly with incomplete inclusion of the correlation and exchange effects which are weakly dependent on Z. In studying the lower states for ions with Z . 40, an expansion into the PT double series on the parameters $1/Z$, αZ (α is the fine structure constant) is often used.

It permits an evaluation of the relative contributions of the different expansion terms: non-relativistic, relativistic, QED contributions as the functions of *Z*. Nevertheless, the serious problems in calculation of the heavy element spectra leads to a necessity of developing new, high exact methods of account for the QED effects, in particular, the Lamb shift (LS), self-energy (SE) part of the Lamb shift, vacuum polarization (VP) contribution, correction on the nuclear finite size for superheavy elements and its account for different spectral properties of these systems (the energies and constants of the hyperfine structure, derivatives of the one-electron characteristics on nuclear radius, nuclear electric quadrupole, magnetic dipole moments etc. (see Refs. [1–19, 45–73])). In this essence it should be given special attention to two very general and important computer systems for relativistic and QED calculations of atomic and molecular properties developed in the Oxford group and known as GRASP ("GRASP", "Dirac"; "BERTHA", "QED", "Dirac") (see [1–19] and references there). In particular, the BERTHA program embodies a new formulation of relativistic molecular structure theory within the framework of relativistic QED. This leads to a simple and transparent formulation of Dirac-Hartree-Fock-Breit (DHFB) self-consistent field equations along with algorithms for molecular properties, electron correlation, and higher order QED effects. The DHFB equations are solved by a direct method based on a relativistic generalization of the McMurchie-Davidson algorithm for molecular integrals that economizes memory requirements and is not significantly more expensive computationally than comparable nonrelativistic calculations [6].

The useful overview of relativistic electronic structure theory is presented in Ref. [1-4] from the point of view of QED. The participation of the negative-energy states in practical calculations is described from complementary points of view, in order to illustrate how they enter into the operation of relativistic mean-field theories. Examples of the implementation of relativistic electronic structure theory are drawn from studies of gauge invariance, many-body PT theory, inner-shell processes, electron momentum spectroscopy, and relativistic density functional theory. Let us note here that these principal moments are accurately taken into account in our theory, presented below. Naturally, a great interest attracts the use of many-body PT and QED in molecular electronic structure theory.

In this chapter we present the basises of the generalized energy approach (Gell-Mann and Low S-matrix formalism) to relativistic calculation of the radia-

tive and autoionization characteristics of atoms and ions. The basises of the relativistic energy approach to one-electron ions have been considered by Labzovsky et al [89]. Originally the energy approach to radiative and autoionization processes in multielectron atoms and ions has been developed by Ivanova-Ivanov et al (see Refs. [90-116]). The generalized gauge-invariant QED version of the energy approach has been further developed by Glushkov-Ivanov-Ivanova (see Refs. [117-160]). The approach is based on the Gell-Mann and Low S-matrix formalism and the gauge-invariant QED PT with using the optimized one-quasiparticle representation and an accurate account of the relativistic, correlation, nuclear, radiative effects [117 -160]. In relativistic case the Gell-Mann and Low formula expressed an energy shift $_{\Delta E}$ through the QED scattering matrix including the interaction with as the photon vacuum field as the laser field. In the last case it has been possible to develop a new effective approach to describe the interaction of atom with the realistic laser field by means of the radiation emission and absorption lines [121-131]. The first case is corresponding to definition of the traditional radiative and autoionization characteristics of multielectron atoms and ions. The Superatom package (the PC complex of Fortran programs) numerically realizes a new method. The wave function zeroth basis is found from the Dirac equation with a potential, which includes the ab initio (the optimized model potential or DF potentials, the electric and polarization potentials of a nucleus; the Gaussian or Fermi forms of the charge distribution in a nucleus are usually used) [117-160]. The correlation corrections of the PT high orders are taken into account within the Green functions method (with the use of the Feynman diagram's technique). All correlation corrections of the second order and dominated classes of the higher orders diagrams (electrons screening, particle-hole interaction, mass operator iterations) are taken into account.

Let us describe the key moments of the energy approach to relativistic calculation of spectra, radiative and autoionization characteristics for the multielectron atoms, multicharged ions with an accurate account of the relativistic, exchange-correlation and other effects **(**details can be found in Refs. [90-160]). Originally the energy approach to radiative and autoionization processes in multielectron atoms and ions has been developed by Ivanova-Ivanov et al (see Refs. [90-116]). The generalized gauge-invariant QED version of the energy approach has been further developed by Glushkov-Ivanov-Ivanova (see Refs. [117,121,128]).

1.3 Definition of basis of relativistic wave functions

As usual, a multielectron atom is described by the Dirac relativistic Hamiltonian (the atomic units are used):

$$H = \sum_i h(r_i) + \sum_{i>j} V\left(r_i r_j\right). \tag{1.1}$$

Here, *h(r)* is one-particle Dirac Hamiltonian for electron in a field of the finite size nucleus and *V* is potential of the inter-electron interaction. In order to take into account the retarding effect and magnetic interaction in the lowest order on parameter α^2 (α is the fine structure constant) one could write [4,16]:

$$V\left(r_i r_j\right) = exp\left(i\omega_{ij} r_{ij}\right) \cdot \frac{\left(1 - \alpha_i \alpha_j\right)}{r_{ij}}, \tag{1.2}$$

where ω_{ij} is the transition frequency; α_i ,α_j are the Dirac matrices. The zeroth order Hamiltonian H_0 операторand perturbation operator can be presented in the standard form as follows [15-19]:

$$H_0 = \sum_i a_i^+ a_i E_i \tag{1.3}$$

$$H_{\text{int}} = \sum_{ij} a_i^+ a_j V_{ij} + \frac{1}{2} \sum_{ijkl} V_{ijkl} a_i^+ a_j^+ a_k a_l \tag{1.4}$$

$$V_{ij} = \int d\vec{r} \cdot \varphi_i\left(\vec{r}\right)\left[-V_C\left(r\right)\right] \cdot \varphi\left(\vec{r}\right) \tag{1.5}$$

$$V_{ijkl} = \iint d\vec{r}_1 d\vec{r}_2 \; \varphi\left(\vec{r}_1\right)\varphi\left(\vec{r}_2\right) V\left(r_1 r_2\right) \varphi_k\left(\vec{r}_2\right) \varphi_l\left(\vec{r}_1\right), \tag{1.6}$$

where $\varphi\left(\vec{r}\right)$ are one-electron functions (Dirac bispinors), E_i – one-electron energies, V_C is the central field self-consistent potential of the Coulomb type. The

latter can be taken in the form of the usual Dirac-Fock potential (with the optimization parameter b; see below) or some model potential, which imitates an effect of the electron subsystem.

In many papers (see Refs.[90-116]) Ivanov-Ivanova effective potential was successfully used in calculations of the spectroscopic characteristics of one-quasiparticle atomic systems (i.e. atoms or ions with one valent electron or vacancy above the closed electron shells atomic core). This potential V_C is usually presented as sum of the potentials, which imitate a contribution of the K,L,M… shells of the N –electron atomic core (in th Coulomb units) [90]:

$$v_K = 2[1-e^{-2rb}(1+rb)]/Zr \tag{1.7a}$$

$$v_L = 8[1-e^{-br}(1+0.75br+0.25b^2r^2+0.0625b^3r^3)]/Zr \tag{1.7b}$$

$$v_M = (N-10)[1-1/(1+br+b^2r^2+b^3r^3)]/Zr \tag{1.7c}$$

The Coulomb units (C.u.) are simply connected with the traditional atomnic units (a.u.) as follows: 1 C.u. length = 1 a.u.Z; 1 C.u. energy = 1 a.u. Z^2. It is important to note that the potential (7) V_C has the proper asymptotics:

$$V_C \to \text{const}, \; dV_C/dr \to 0 \;\; \text{for} \;\; r \to 0, \tag{1.8a}$$

$$V_C \to N/rZ \;\; \text{for} \;\; r \to \infty. \tag{1.8b}$$

The proper asymptotical behaviour of V_C under $r \to 0$ is of a great importance for correct definition of position of the quasiparticle orbital nodes and précised calculation of the transition probabilities, oscillator strengths, radiation widths etc.

The Dirac equation potential can also include the electric and polarization potentials of a nucleus and exchange-correlation potentials. The usual exact account of the exchange corrections is provided by using the Dirac-Fock exchange potential. The alternative Kohn-Sham (KS) exchange potential is as follows [29]:

$$V_X^{KS}(r) = -(1/\pi)[3\pi^2\rho(r)]^{1/3}. \quad (1.9)$$

In the local density approximation of the density functional theory (DFT) the relativistic potential is:

$$V_X[\rho(r), r] = \frac{\delta E_X[\rho(r)]}{\delta\rho(r)}, \quad (1.10)$$

where $E_X[\rho(r)]$ is the exchange energy of the multielectron system corresponding to the homogeneous density $\rho(r)$, which is obtained from a Hamiltonian having a transverse vector potential describing the photons. In this theory the exchange potential is [33,119]:

$$V_X[\rho(r), r] = V_X^{KS}(r) \cdot \{\frac{3}{2}\ln\frac{[\beta + (\beta^2+1)^{1/2}]}{\beta(\beta^2+1)^{1/2}} - \frac{1}{2}\}, \quad (1.11)$$

where

$$\beta = [3\pi^2\rho(r)]^{1/3} / c\,. \quad (1.12)$$

Here c is the light velocity. The corresponding correlation functional is [29-33]:

$$V_C[\rho(r), r] = -0.0333 \cdot b \cdot \ln[1 + 18.3768 \cdot \rho(r)^{1/3}], \quad (1.13)$$

where *b* is the optimization parameter (for details see Refs. [119,121]).
The differential equations for the radial functions *F* and *G* (components of the Dirac spinor) are:

$$\frac{\partial F}{\partial r} + (1+\chi)\frac{F}{r} - (\varepsilon + m - V)G = 0, \quad (1.14a)$$

$$\frac{\partial G}{\partial r} + (1-\chi)\frac{G}{r} + (\varepsilon - m - V)F = 0, \quad (1.14b)$$

where *F*, *G* are the large and small components respectively; χ is the quantum number. At large χ, the functions *F* and *G* vary rapidly at the origin. One could write:

$$F(r), G(r) \approx r^{\gamma-1}, \ \gamma = \sqrt{\chi^2 - \alpha^2 z^2} \ . \qquad (1.15)$$

This creates difficulties in numerical integration of the equations in the region $r \to 0$. To prevent the integration step from becoming too small it is usually convenient to turn to new functions isolating the main power dependence:

$$f = Fr^{1-|\chi|} \ ,$$
$$g = Gr^{1-|\chi|} \ . \qquad (1.16)$$

The Dirac equations for *F* and *G* components are transformed as follows:

$$f' = -(\chi + |\chi|) f / r - \alpha Z V g - (\alpha Z E_{n\chi} + 2/\alpha Z) g, \qquad (1.17a)$$

$$g' = (\chi - |\chi|) g / r - \alpha Z V f + \alpha Z E_{n\chi} f . \qquad (1.17b)$$

Here $E_{n\chi}$ is one-electron energy without the rest energy. The boundary values are defined by the first terms of the Taylor expansion:

$$g = \left(V(0) - E_{n\chi}\right) r \alpha Z / (2\chi + 1); \quad f = 1 \text{ at } \chi < 0 , \qquad (1.18a)$$

$$f = \left(V(0) - E_{n\chi} - 2/\alpha^2 Z^2\right) \alpha Z; \quad g = 1 \text{ at } \chi > 0 . \qquad (1.18b)$$

The condition *f*, $g \to 0$ at $r \to \infty$ determines the quantified energies of the state $E_{n\chi}$. The system of equations (18) is numerically solved by the Runge-Kutt method (the separated block in the "Superatom" package [90-160]).

The self-consistence condition of the continuum state functions means that the normalized functions differ by less than 10^{-6} in relation to their values at the maximum point on two neighbour iterations.

1.4 Nuclear finite size and radiation QED effects

In order to account for the nuclear finite size effect one could describe the charge distribution in the nucleus $\rho(r)$ by the following Gaussian function:

$$\rho\left(r\middle|R\right)=\left(4\gamma^{3/2}/\sqrt{\pi}\right)\exp\left(-\gamma r^{2}\right), \tag{1.19}$$

$$\int_{0}^{\infty}drr^{2}\rho\left(r\middle|R\right)=1;\quad\int_{0}^{\infty}drr^{3}\rho\left(r\middle|R\right)=R, \tag{1.20}$$

where $\gamma=4/\pi R^{2}$, and R is the effective nuclear radius. The following simple dependence of R on Z is assumed: $R=1.606\cdot10^{-13}\cdot Z^{1/3}$ (cm). Such a definition of R is rather conventional. We assume it as some zeroth approximation. The Coulomb potential for the spherically symmetric density $\rho(r|R)$ is:

$$V_{nucl}\left(r\middle|R\right)=-\left((1/r)\int_{0}^{r}dr'r'^{2}\rho\left(r'\middle|R\right)+\int_{r}^{\infty}dr'r'\rho\left(r'\middle|R\right)\right). \tag{1.21}$$

It is determined by the following system of differential equations [4]:

$$V_{nucl}'\left(r,R\right)=\left(1/r^{2}\right)\int_{0}^{r}dr'r'^{2}\rho\left(r',R\right)\equiv\left(1/r^{2}\right)y\left(r,R\right),$$

$$y'\left(r,R\right)=r^{2}\rho\left(r,R\right),$$

$$\rho'\left(r,R\right)=-8\gamma^{5/2}r/\sqrt{\pi}\exp\left(-\gamma r^{2}\right)=-2\gamma r\rho\left(r,R\right)=-\frac{8r}{\pi r^{2}}\rho\left(r,R\right), \tag{1.22}$$

with the boundary conditions:

$$V_{nucl}\left(0,R\right)=-4/\left(\pi r\right),\ y\left(0,R\right)=0,$$
$$\rho\left(0,R\right)=4\gamma^{3/2}/\sqrt{\pi}=32/R^{3}. \tag{1.23}$$

The presented nuclear model was earlier used in many calculations of the atomic and nuclear systems [128-160]. It can be improved where necessary. Moreover, any relativistic mean field model, nuclear DFT, the HF theory with density dependent forces etc may be here used [119,131-135].

The procedure for taking into account the QED corrections is given in Refs. [3,4,12,90,109]. Procedure for an account of the radiative QED corrections is in details given in the refs. [15-18]. Regarding the vacuum polarization effect let us note that this effect is usually taken into account in the first PT theory order by means of the Uehling potential. This potential is usually written as follows [15,90]):

$$U(r) = -\frac{2\alpha}{3\pi r}\int_1^\infty dt\,\exp\left(-2rt/\alpha Z\right)\left(1+1/2t^2\right)\frac{\sqrt{t^2-1}}{t^2} \equiv -\frac{2\alpha}{3\pi r}C(g), \quad (1.24)$$

where $g=r/\alpha Z$. In our calculation we usually use more exact approach. The Uehling potential, determined as a quadrature (1.24) may be approximated by a simple analytical function with high precision. The use of new approximation of the Uehling potential permits one to decrease the calculation errors for this term down to 0.5 – 1%. The detailed description of this approximation and calculation scheme of the Lamb shift self-energy part is given in Refs. [3,4,15-18,90,109]. The alternative potential approach to account of the radiative self-energy corrections is based on using the corresponding radiative potentials (see refs. [45-58]).

1.5 The one-particle optimized gauge-invariant representation

The problem of the searching for the optimal one-electron representation is one of the oldest in the theory of multielectron atoms. Two decades ago Davidson had pointed the principal disadvantages of the traditional representation based on the self-consistent field approach and suggested the optimal "natural orbitals" representation. Nevertheless there remain insurmountable calculational difficulties in the realization of the Davidson program. One of the simplified recipes represents, for example, the DFT method [29-33].

Unfortunately, this method doesn't provide a regular refinement procedure in the case of the complicated atom with few quasiparticles (electrons or vacancies besides the core of closed shells). Our density functional method, based on the formally exact QED PT, uses for this purpose the model bare potential, constructed with accounting for the spectroscopic information concerning simplest systems with one quasiparticle [90].

In the theory of radiative and nonradiative decay of the quasistationary states of a multielectron atom it is well known an energy approach (see below) , based on the adiabatic Gell-Mann and Low formula [89,117,128] for the energy shift δE with electrodynamic scattering matrice. The method is a consistently electrodynamic one, allowing for the uniform consideration of a variety of induced and spontaneous processes different by their physical nature [129-156].

For simplicity, let us consider now the one-quasiparticle system. The multiquaiparticle case doesn't contain principally new moments. In the lowest, second order, of the QED PT for the δE there is the only one- quasiparticle Feynman diagram A (fig.1.1), contributing the Im δE (the radiation decay width).

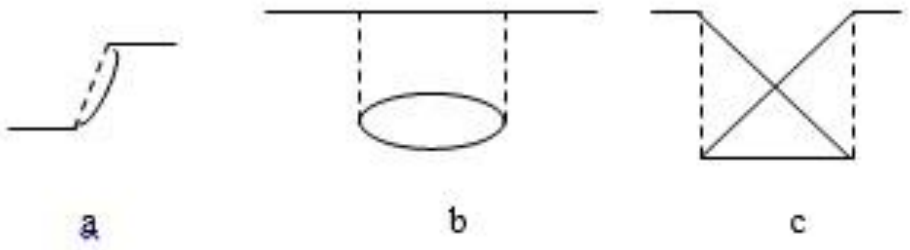

Figure 1.1 a: second other EDPT diagram contributing the imaginary energy part related to the radiation transitions. b and c: fourth order polarization diagrams.

In the next, the fourth order there appear diagrams, whose contribution into the ImδE account for the core polarization effects. This contribution describes collective effects and it is dependent upon the electromagnetic potentials gauge (the gauge noninvariant contribution). Let us examine the multielectron atom with one quasiparticle in the first excited state, connected with the ground state by the radiation transition. In the zero QED PT ap-

proximation we, as usually (see ref.[128]), use the one electron bare potential:

$$V_N(r)+V_C(r), \tag{1.25}$$

with $V_N(r)$ describing the electric potential of the nucleus, $V_C(r)$, imitating the interaction of the quasiparticle (initial or any other appearing in the real and virtual processes) with the core of closed shells. The perturbation in terms of the second quantization representation reads

$$-V_C(r)\ \psi^+(r)\ \psi(r)\ -\ j_\mu(x)\,A^\mu(x) \tag{1.26}$$

The core potential $V_C(r)$ is related to the core electron density $\rho_C(r)$ in a standard way. The latter fully defines the one electron representation. Moreover, all the results of the approximate calculations are the functionals of the density $\rho_C(r)$. Here, the lowest order multielectron effects, in particular, the gauge dependent radiative contribution for the certain class of the photon propagator calibration is treating. This value is considered to be the typical representative of the electron correlation effects, whose minimization is a reasonable criteria in the searching for the optimal one-electron basis of the PT. Besides, this procedure derives an undoubted profit in the routine spectroscopic calculations as it provides the way of the refinement of the atomic characteristics calculations, based on the "first principles" . Remember that the closeness of the radiation probabilities calculated with the alternative forms of the transition operator is commonly used as a criterion of the multielectron calculations quality. It is of special interest to verify the compatibility of the new optimization principle with the other requirements conditioning a "good" one-electron representation.

The imaginary part of the diagram a (fig.1.1) contribution in the case of the Lorentz calibration has been presented previously as a sum of the partial contributions of α-s transitions from the initial state α to the final state s [3,128],

$$\mathrm{Im}\delta E_\alpha\,(\mathrm{a}) = \sum_s\ \mathrm{Im}\ \delta E\ (\alpha\text{-}s;\ \mathrm{a}). \tag{1.27}$$

Two fourth order polarization diagrams b,c (fig.1.1) are considered in this article. The contributions being under consideration, are gauge- dependent, though the results of the exact calculation of any physical quantity must be gauge independent . All the noninvariant terms are multielectron by their nature. Let us take the photon propagator calibration as follows:

$$D = D_{\mathrm{T}} + CD_{\mathrm{L}},$$

$$D_{\mathrm{T}} = \delta_{\mu\nu} / (k_0^2 - k^2),$$

$$D_{\mathrm{L}} = - k_\mu k_\nu / (k_0^2 - k^2). \qquad (1.28)$$

Here, D_{T} represents the exchange of electrons by transverse photons, D_{L} that by longitudinal ones. The values C=0 and C=1 of the gauge constant are related to the Lorentz and to the Landau calibrations correspondingly. One could calculate the contribution of the a,b,c diagrams (fig.1.1) into the Im δE taking into account both the D_{T} and D_{L} parts. The A diagram contribution into the Im δE related to the α -s transition reads as

$$-\frac{e^2}{8\pi}\int\int \mathrm{d}r_1\mathrm{d}r_2\,\psi_\alpha^+(r_1)\;\psi_s^+(r_2)\;\frac{1-\alpha_1\alpha_2}{r_{12}}\sin(\omega_{\alpha s} r_{12})\;\psi_\alpha(r_2)\;\psi_s(r_1), \quad (1.29)$$

for $D = D_{\mathrm{T}}$, and

$$-\frac{e^2}{8\pi}\int\int \mathrm{d}r_1\,\mathrm{d}r_2\;\psi_\alpha^+(r_1)\;\psi_s^+(r_2)\;\{[(1-\alpha_1 n_{12}\,\alpha_2 n_{12})/ r_{12}]\sin(\omega_{\alpha s} r_{12})+\omega_{\alpha s}\,(1+$$

$$+\;\alpha_1 n_{12}\alpha_2 n_{12})\times\cos(\omega_{\alpha s} r_{12})\}\,\psi_\alpha(r_2)\,\psi_s(r_1), \qquad (1.30)$$

for D=D_{L}, where $\omega_{\alpha s}$ is the α -s transition energy. According to the Grant theorem [1], the $D_{\mu\nu,\mathrm{L}}$ contribution vanishes, if the one-quasiparticle functions ψ_α , ψ_s satisfy the same Dirac equation. Nevertheless this term is to be retained when using the distorted waves approximation, for example. Another very important example represents the formally exact approach based on the bare hamiltonian defined by its spectrum without specifying its analytic form [129,130]. Here the noninvariant contribution appears already in the lowest or-

der. When calculating the forth order contributions some approximations are inevitable. These approximations have been formulated in Refs.[90, 94,96], where the polarization corrections to the state energies have been considered. Here, we reproduce briefly the calculational scheme. Let us consider the direct polarization diagram as an example.

After the linearization over the gauge constant *C*, the formal expression for the sought for value looks as:

$$Im\delta E_{ninv}(\alpha - s \mid b) = -C\frac{e^2}{4\pi}\int\int\int\int dr_1 dr_2 dr_3 dr_4 \sum_{n>f,\, m\le f}\left(\frac{1}{\omega_{mn}+\omega_{\alpha s}}+\frac{1}{\omega_{mn}-\omega_{\alpha s}}\right)$$

$$\times\Psi^+_\alpha(r_1)\Psi^+_m(r_2)\Psi^+_s(r_4)\Psi^+_n(r_3)\cdot[(1-\alpha_1\alpha_2)/r_{12}]\cdot\{[\alpha_3\alpha_4-(\alpha_3 n_{34})(\alpha_4 n_{34})]/r_{34}$$

$$\times\sin[\omega_{\alpha n}(r_{12}+r_{34})]+[1+(\alpha_3 n_{34})(\alpha_4 n_{34})]\omega_{\alpha n}\cos[\omega_{\alpha n}(r_{12}+r_{34})]\}$$

$$\times\Psi_m(r_3)\Psi_\alpha(r_4)\Psi_n(r_2)\Psi_s(r_1). \qquad (1.31)$$

and the upper continuum electron states; $m \le f$ indicates the finite number of states in the core and the states of the negative continuum (accounting for the electron vacuum polarization). All the vacuum polarization and the self-energy corrections to the sought for values are omitted. Their numerical smallness compared with the other relativistic corrections to the different atomic characteristics had been verified by the numerous calculations. The renormalization procedure is not needed here. Nevertheless the second-order vacuum polarization and self-energy corrections can be additively added to the complex state energy. The remaining expression includes summation over the bound and upper continuum atomic states. To evaluate this sum, we use the analytic relation between the atomic electron Fermi level and the core electron density $\rho_c(r)$, appropriate to the homogeneous nonrelativistic electron gas (the Tomas- Fermi approximation). Now the sum $\sum_{n>f,\, m<f}$ can be calculated analytically , its value becomes a functional of the core electron density. The resulting expression looks as the correction due to the additional nonlocal interaction of the active quasiparticle with the closed shells. Nevertheless its calculation is reducible to the solving of the system of the ordinary differential equations - the one- dimensional procedure. The most important refinements can be introduced by accounting for the relativistic and the density gradient

corrections to the Tomas- Fermi formula (see Refs. [3,4]). The same program is realized for the remaining forth order QED PT polarization corrections. The minimization of the functional Im δE_{ninv} (b+c) leads to the integro- differential equation for the ρ_c (the Dirac-Fock or Dirac-Kohn-Sham-like equations for the electron density) that can be solved using one of the standard numerical codes. As a result one can get the optimal PT one-quasi-particle basis. In concrete calculations it is sufficient to use a more simplified procedure, which is reduced to the functional minimization using the variation of the correlation potential parameter *b* in Eq. (13) or (17) [3,4,117,128].

1.6 Energy approach to calculating radiative transition probabilities

1.6.1 General remarks

The energy approach to the calculation of the radiation widths has been originally proposed by Ivanov-Ivanova and coworkers [90-116]. In general, this approach permits combined consideration of different atomic processes on the basis of a consistently relativistic theory. Thus, the tedious procedure of phase convention in calculating the matrix elements of different operators is avoided, although the final formulae, of course, must coincide with the formulae obtained using the traditional method operating with the amplitudes of the processes, which is usually called as the amplitude method. The energy approach simplifies the analysis of complex atomic processes including processes with the interference of different kinds of channels (i.e. radiation and autoionization ones). More advance QED version of the energy approach has been developed by Glushkov-Ivanova-Ivanov (see, for example, Refs. [117-128]) and based on the Gell-Mann and Low S-matrix formalism and gauge-invariant QED PT. The advanced approach provides absolutely ab initio treating different atomic processes, including radiative transitions and autoionization processes, within the consistent QED theory. Moreover, the corresponding advances approaches have been developed in order to solve many actual problems of the laser-atom interaction, nuclear physics, ions collision problems etc (see Refs. [147-160]).

Generally speaking, the majority of complex atomic systems possesses a dense energy spectrum of interacting states with essentially relativistic proper-

ties. 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 [161]. In constructing *M*, the Gell-Mann and Low adiabatic formula for ΔE is used. A similar approach, using the Gell-Mann and Low formula with the electrodynamic scattering matrix, is applicable in the relativistic atom theory [89]; the approach is consistently electrodynamic. In contrast to the non-relativistic case, the secular matrix elements are already complex in the second order of the electrodynamic PT (first order of the interelectron interaction). Their imaginary parts are connected with the radiation decay (radiation) possibility.

The total energy shift of the state is usually presented in the form:

$$\Delta E = \mathrm{Re}\,\Delta E + i\,\mathrm{Im}\,\Delta E \qquad \mathrm{Im}\,\Delta E = -\Gamma/2 \tag{1.32}$$

where Γ is interpreted as the level width, and the decay possibility $P = \Gamma$.

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 [90-94,105-110,117-121] 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 ΔE. 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 [12,90,94]:

$$M = M^{(0)} + M^{(1)} + M^{(2)} + M^{(3)}. \tag{1.33}$$

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 (35) one could have summarised 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 [90-98,117-128] using Feynman diagrams. 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. 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 can be approximated as follows:

$$M = \tilde{M}^{(1)} + \tilde{M}^{(2)} \tag{1.34}$$

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 note that in the QED theory, the photon propagator D(12) plays the role of this interaction. Naturally (see above) the analytical form of D(12) depends on the gauge, in which the electrodynamic potentials are written. 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 photoprocesses in the approximate calculations is a well known fact and is in

details investigated by Grant, Armstrong, Aymar and Luc-Koenig, Glushkov-Ivanov [1-4,128]. 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 photoprocesses are gauge invariant. 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 QED version of the energy approach (see above part 2.4).

1.6.2 Imaginary part of the secular matrix

As it has been indicated (see Eq.(2)) in the QED PT second order the relativistic and radiation effects are taken into account exchanging the interelectron non-relativistic $1/Zr_{12}$ interaction with the operator (2). The radiation processes are determined by the imaginary part of the interaction (2) between the active quasiparticle and the electrodynamic vacuum of the electronic field. The presence of the polarizable core can be effectively accounted for by modification of (2). This corresponds to a modification of the radiation transition operator in the traditional amplitude approach. A local form of the modified transition operator has been previously treated by Hibbert, Migdalec, Ivanova-Ivanov, Glushkov et al (see Refs. [78,82,93,94,117-128]). An integral form of the additional polarization interaction, including the imaginary part, has been deduced on the base of the analysis of the second-order (the QED PT fourth order) polarization diagrams (fig.1.1 b,c). In result one could take into account for the corresponding corrections to $\mathrm{Im}\Delta E$. The detailed description of the accounting for the correlation corrections of the PT high orders within the Green functions method (with the use of the Feynman diagram's technique) is given in Refs. [93,94] (see also Refs. [3,4,117-128], where additional details can be found).

The probability is directly connected with imaginary part of electron energy of the system, which is defined in the lowest order of perturbation theory as follows:

$$\mathrm{Im}\Delta E(a;\, fig.1) = -\frac{e^2}{4\pi} \sum_{\substack{\alpha>n>f \\ [\alpha<n\le f]}} V_{\alpha n \alpha n}^{|\omega_{\alpha n}|}\,, \qquad (1.35)$$

where $\sum_{\alpha>n>f}-$ for electron and $\sum_{\alpha<n\le f}-$ for vacancy. The potential V is as follows:

$$V_{ijkl}^{|\omega|}=\iint dr_1 dr_2 \Psi_i^*(r_1)\Psi_j^*(r_2)\frac{\sin|\omega|r_{12}}{r_{12}}(1-\alpha_1\alpha_2)\Psi_k^*(r_2)\Psi_l^*(r_1) \qquad (1.36)$$

The separated terms of the sum in (38) represent the contributions of different channels and a probability of the dipole transition is:

$$\Gamma_{\alpha_n}=\frac{1}{4\pi}\cdot V_{\alpha_n\alpha_n}^{|\omega_{\alpha_n}|} \qquad (1.37)$$

The corresponding oscillator strength :

$$gf=\lambda_g^2\cdot\Gamma_{\alpha_n}/6.67\cdot 10^{15}, \qquad (1.38)$$

where g is the degeneracy degree, λ is a wavelength in angstroms (Å). Under calculating the matrix elements (38) one could use the angle symmetry of the task and write the expansion for potential $\sin|\omega|r_{12}/r_{12}$ on spherical functions as follows:

$$\frac{\mathbf{sin}|\omega|r_{12}}{r_{12}}=\frac{\pi}{2\sqrt{r_1 r_2}}\sum_{\lambda=0}^{\infty}(\lambda)J_{\lambda+1/2}(|\omega|r_1)J_{\lambda+1/2}(|\omega|r_2)\widehat{P_\lambda}(\mathbf{cos}\boldsymbol{r}_1\boldsymbol{r}_2), \qquad (1.39)$$

where J –is the Bessel function of first kind and $(\lambda) = 2\lambda + 1$. This expansion is corresponding to usual multipole one for probability of radiative decay. Substitution of the expansion (41) to matrix element of interaction gives as follows:

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

$$Q_\lambda=Q_\lambda^{\mathrm{Qul}}+Q_\lambda^{\mathrm{Br}}. \qquad (1.40)$$

where j_i are the entire single electron momentums, m_i – their projections; Q_λ^{Cul} and Q_λ^{Br} are connected with the Coulomb $(1/Zr_{12})$ and Breit magnetic $(-\alpha_1\alpha_2/Zr_{12})$ parts of the operator (2). The total radiation width of the one-quasiparticle state is presented in the form:

$$\begin{aligned}\Gamma(\gamma) &= -2\,\mathrm{Im}\,M^1(\gamma) = -2\sum_{\lambda n l j}(2j+1)\,\mathrm{Im}\,Q_\lambda\left(n_\gamma l_\gamma j_\gamma nlj\right)\\ Q_\lambda &= Q_\lambda^{Cul} + Q_\lambda^{Br}.\end{aligned} \tag{1.41}$$

The individual terms of the $\sum_{nlj}$ sum correspond to the partial contribution of the $n_\lambda l_\lambda j_\lambda \to nlj$ transitions; $\sum_\lambda$ is a sum of the contributions of the different multiplicity transitions. The detailed expressions for the Coulomb and Breit parts can be found in Refs. [11-16]. The imaginary part Q_λ^{Cul} contains the radial R_λ and angular S_λ integrals as follows:

$$\begin{aligned}\mathrm{Im}\,Q_\lambda^{Cul}(12;43) = Z^{-1}\,\mathrm{Im}\{&R_\lambda(12;43)S_\lambda(12;43) + R_\lambda(\tilde{1}2;4\tilde{3})S_\lambda(\tilde{1}2;4\tilde{3}) +\\ &+R_\lambda(1\tilde{2};\tilde{4}3)S_\lambda(1\tilde{2};\tilde{4}3) + R_\lambda(\tilde{1}\tilde{2};\tilde{4}\tilde{3})S_\lambda(\tilde{1}\tilde{2};\tilde{4}\tilde{3})\}.\end{aligned} \tag{1.42}$$

In the non-relativistic limit there remains only the first term in (44) depending only on the large component $f(r)$ of the one-electron Dirac functions:

$$\begin{aligned}\mathrm{Im}\,R_\lambda(12;43) &= \frac{1}{2}(2\lambda+1)\pi X_\lambda(13)X_\lambda(24)\\ X_\lambda(12) &= \int dr\, r^{3/2}\, f_1(r)\,J^{(1)}_{\lambda+1/2}\left(r\alpha Z|\omega|\, f_2(r)\right)\end{aligned} \tag{1.43}$$

The angular coefficient has only a real part:

$$S_\lambda(12;43) = S_\lambda(13)S_\lambda(24) \qquad S_\lambda(13) = \{\lambda l_1 l_3\}\begin{pmatrix} j_1 & j_3 & \lambda\\ \frac{1}{2} & -\frac{1}{2} & 0\end{pmatrix} \tag{1.44}$$

$\{\lambda l_1 l_3\}$ means that λ, 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 (44) 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 $j_i > l_i$. Only the phase factor of the formulae (43)-(45) depends on the orbital momenta l_i. Such a simple form of the angular part of the matrix elements has been derived by Kanjauskas and Rudzikas (1975; see Refs. [3,4,90-94]) when calculating $\mathrm{Re}\,\Delta E$.
The Breit (magnetic) part can be expressed as follows:

$$Q_\lambda^{Br} = Q_{\lambda,\lambda-1}^{Br} + Q_{\lambda,\lambda}^{Br} + Q_{\lambda,\lambda+1}^{Br} \tag{1.45}$$

The corresponding imaginary part (47) is as follows [90]:

$$\begin{aligned} \mathrm{Im}\, Q_{\lambda,l}^{Br} = \frac{1}{Z}\mathrm{Im}\{ & R_\lambda\left(12;\tilde{4}\tilde{3}\right) S_\lambda^l\left(12;\tilde{4}\tilde{3}\right) + R_\lambda\left(\tilde{1}\tilde{2};43\right) S_\lambda^l\left(\tilde{1}\tilde{2};43\right) + \\ & + R_\lambda\left(\tilde{1}2;\tilde{4}3\right) S_\lambda^l\left(\tilde{1}2;\tilde{4}3\right) + R_\lambda\left(\tilde{1}\tilde{2};\tilde{4}\tilde{3}\right) S_\lambda^l\left(\tilde{1}\tilde{2};\tilde{4}\tilde{3}\right)\}. \end{aligned} \tag{1.46}$$

The angular part S_λ^l has the form

$$S_\lambda^l(12;43) = (2\lambda+1) S_\lambda^l(13) S_\lambda^l(24) (-1)^{\lambda+l+1} \tag{1.47}$$

$$\begin{aligned} S_\lambda^l(12) = (-1)^{l_2+j_2} \{l l_1 l_3\} & \begin{pmatrix} j_2 & j_i & \lambda \\ -\frac{1}{2} & \frac{1}{2} & 0 \end{pmatrix} \times \left(\frac{1}{\left[2\lambda(\lambda+1)\right]^{1/2}} [(-1)^{j_1+j_2+\lambda}(2j_2+1) + \right. \\ & \left. + (2j_1+1)] \begin{pmatrix} \lambda & 1 & l \\ -1 & 1 & 0 \end{pmatrix} + (-1)^{l_2+j_1+\lambda} \begin{pmatrix} \lambda & 1 & l \\ 0 & 0 & 0 \end{pmatrix} \right) \end{aligned} \tag{1.48}$$

The total probability of a λ - pole transition is usually represented as a sum of the electric P_λ^E and magnetic P_λ^M parts. The electric (or magnetic) λ - pole transition $\gamma \to \delta$ connects two states with parities which by λ (or λ +1) units. In our designations

$$P_\lambda^E(\gamma\to\delta)=2(2j+1)Q_\lambda^E(\gamma\delta;\gamma\delta)\qquad Q_\lambda^E=Q_\lambda^{Cul}+Q_{\lambda,\lambda-1}^{Br}+Q_{\lambda,\lambda+1}^{Br}$$
$$P_\lambda^M(\gamma\to\delta)=2(2j+1)Q_\lambda^M(\gamma\delta;\gamma\delta)\qquad Q_\lambda^M=Q_{\lambda,\lambda}^{Br}. \tag{1.49}$$

In the numerical calculations the transition probability , as usually, is expanded to the series on the known parameter $\alpha\omega$ as follows:

$$Q_\lambda^{Qul}\approx(\alpha\omega)^{(\lambda)},\ Q_{\lambda,\lambda-1}^{Br}\approx(\alpha\omega)^{\lambda},\ Q_{\lambda\lambda}^{Br}\approx(\alpha\omega)^{\lambda+3},\ Q_{\lambda,\lambda+1}\approx(\alpha\omega)^{\lambda+5}. \tag{1.50}$$

In a case of the two-quasi-particle states (this case of the Ne-like ions, where the excited states are represented as stales with the two quasiparticles – electron and vacancy above the closed shells core $1s^22s^22p^6$) the corresponding probability has the following form (say, transition: $j_1 j_2[J]\to\bar{j}_1 j_2[\bar{J}]$):

$$P(\lambda\mid j_1 j_2[J],\bar{j}_1 j_2[\bar{J}])=(\bar{J})\begin{Bmatrix}\lambda\ldots J\ldots\bar{J}\\ j_2\cdots\bar{j}_1\cdots j_1\end{Bmatrix}P(\lambda\mid 1\,\bar{1})(\bar{j}_1), \tag{1.51}$$

where the electric and magnetic parts are defined above.

1.6.3 Energy approach to calculating autoionization widths for atoms

The autoionization (Auger) width and, accordingly, the autoionization decay probability are defined by the square of an electron interaction matrix element having the form [90-94,117,128]:

$$V_{1234}^{\omega}=[(j_1)(j_2)(j_3)(j_4)]^{1/2}\sum_{\lambda\mu}(-1)^{\mu}\begin{pmatrix}j_1 j_3 & \lambda\\ m_1-m_3 & \mu\end{pmatrix}\times\mathrm{Re}\,Q_\lambda(1234) \tag{1.52}$$

The real part of the electron interaction matrix element is determined using expansion in terms of Bessel functions: :

$$\frac{\cos|\omega|r_{12}}{r_{12}} = \frac{\pi}{2\sqrt{r_1 r_2}} \sum_{\lambda=0} (\lambda) J_{\lambda+1/2}(|\omega| r_<) J_{-\lambda-1/2}(|\omega| r_>) P_\lambda(\cos \mathbf{r}_1 \mathbf{r}_2). \quad (1.53)$$

The Coulomb part Q_λ^{Qul} is expressed in terms of radial integrals R_λ, angular coefficients S_λ:

$$\begin{aligned} \mathrm{Re}\, Q_\lambda^{\mathrm{Qul}} = \frac{1}{Z} \mathrm{Re}\{ & R_l(1243) S_\lambda(1243) + R_\lambda(\tilde{1}24\tilde{3}) S_\lambda(\tilde{1}24\tilde{3}) \\ & + R_\lambda(1\tilde{2}\tilde{4}3) S_\lambda(1\tilde{2}\tilde{4}3) + R_\lambda(\tilde{1}\tilde{2}\tilde{4}\tilde{3}) S_\lambda(\tilde{1}\tilde{2}\tilde{4}\tilde{3})\}. \end{aligned} \quad (1.54)$$

As a result, the autoionization decay probability is expressed in terms of $\mathrm{Re}Q_\lambda(1243)$ matrix elements :

$$\mathbf{Re}\, R_\lambda(1243) = \iint dr_1 r_1^2 r_2^2 f_1(r_1) f_3(r_1) f_2(r_2) f_4(r_2) Z_\lambda^{(1)}(r_<) Z_\lambda^{(1)}(r_>). \quad (1.55)$$

where f is the large component of radial part of single electron state Dirac function and function Z is :

$$Z_\lambda^{(1)} = \left[\frac{2}{|\omega_{13}|\alpha Z} \right]^{\lambda+1/2} \frac{J_{\lambda+1/2}(\alpha|\omega_{13}|r)}{r^\lambda \Gamma(\lambda + 3/2)}. \quad (1.56)$$

The angular coefficient is defined by standard way as above [3]. The Breit part of Q is defined in the similar way as above, but the contribution of our interest is a real part. The Breit interaction is known to change considerably the Auger decay dynamics in some cases (see, for example, Refs. [93]).

The calculation of radial integrals $\mathbf{Re}R_\lambda(1243)$ is reduced to the solution of a system of differential equations [93]:

$$\left.\begin{aligned} y_1' &= f_1 f_3 Z_\lambda^{(1)}(\alpha|\omega|r) r^{2+\lambda}, \\ y_2' &= f_2 f_4 Z_\lambda^{(1)}(\alpha|\omega|r) r^{2+\lambda}, \\ y_3' &= [y_1 f_2 f_4 + y_2 f_1 f_3] Z_\lambda^{(2)}(\alpha|\omega|r) r^{1-\lambda}. \end{aligned}\right\} \qquad (1.57)$$

In addition, $y_3(\infty)=\mathbf{Re}R_\lambda(1243)$, $y_1(\infty)=X_\lambda(13)$. The system of differential equations includes also equations for functions $f/r^{|æ|-1}$, $g/r^{|æ|-1}$, $Z_\lambda^{(1)}$, $Z_\lambda^{(2)}$. The formulas for the autoionization (Auger) decay probability include the radial integrals $R_\alpha(\alpha k\gamma\beta)$, where one of the functions describes electron in the continuum state. When calculating this integral, the correct normalization of the function Ψ_k is a problem. The correctly normalized function should have the following asymptotic at $r\to 0$:

$$\left.\begin{matrix} f \\ g \end{matrix}\right\} \to (\lambda\omega)^{-1/2} \begin{cases} \left[\omega + (\alpha Z)^{-2}\right]^{-1/2} \sin(kr+\delta), \\ \left[\omega - (\alpha Z)^{-2}\right]^{-1/2} \cos(kr+\delta). \end{cases} \qquad (1.58)$$

When integrating the master system, the function is calculated simultaneously:

$$N(r) = \left\{\pi\omega_k \left[f_k^2 \left[\omega_k + (\alpha Z)^{-2}\right] + g_k^2 \left[\omega_k + \left(\alpha Z^{-2}\right)\right]\right]\right\}^{-1/2}. \qquad (1.59)$$

It can be shown that at r $\to \infty$, $N(r)\to N_k$, where N_k is the normalization of functions f_k, g_k of continuous spectrum satisfying the condition (1.60).

At last, let us 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 $\mathrm{Re}\,M$ should be diagonalized. The imaginary part is converted by means of the matrix of eigenvectors $\{C_{mk}\}$, obtained by diagonalization of $\mathrm{Re}\,M$:

$$\mathrm{Im}\, M_{mk} = \sum_{ij} C^{*}_{mi}\, M_{ij}\, C_{jk} \tag{1.60}$$

M_{ij} are the matrix elements in the *jj*-coupling scheme, and M_{mk} in the intermediate coupling scheme representation. This procedure is correct to terms of the order of $\mathrm{Im}\, M / \mathrm{Re}\, M$ [128].

References

1. Glushkov A.V., Advanced Relativistic Energy Approach to Radiative Decay Processes in Multielectron Atoms and Multicharged Ions// Quantum Systems in Chemistry and Physics: Progress in Methods and Applications. Series: Progresss in Theoretical Chemistry and Physics, Eds. K.Nishikawa, J. Maruani, E.Brandas, G. Delgado-Barrio, P.Piecuch (Berlin, Springer).-2013-Vol.26.-P.231-254;
2. Khetselius O.Yu., Relativistic energy approach to cooperative electron-gamma-nuclear processes: NEET Effect// Quantum Systems in Chemistry and Physics: Progress in Methods and Applications. Series: Progresss in Theoretical Chemistry and Physics, Eds. K.Nishikawa, J. Maruani, E.Brandas, G. Delgado-Barrio, P.Piecuch (Berlin, Springer).-2012-Vol.26.-P.217-230.
3. K.G. Dyall, K. Faegri, Jr. *Introduction to Relativistic Quantum Theory* (Oxford University Press, Oxford, 2007); I.P. Grant, *Relativistic Quantum Theory of Atoms and Molecules, Theory and Computation, Springer Series on Atomic, Optical, and Plasma Physics*, vol. 40 (Springer, Berlin, 2007), p. 587–626
4. A.V. Glushkov, *Relativistic and Correlation Effects in Spectra of Atomic Systems* (Nauka, Moscow-Odessa, 2006), 550p.
5. A.V. Glushkov, *Relativistic Quantum Theory. Quantum Mechanics of Atomic Systems* (Astroprint, Odessa, 2008), 900p.
6. I.P. Grant, H.M. Quiney, Int. J. Quant. Chem**. 80**, 283–297 (2000) ; K.L. Bell, K.A. Berrington, D.S.F. Crothers, A. Hibbert, K.T. Taylor, *Bertha: 4-Component Relativistic Molecular Quantum Mechanics, in Supercomputing, Collision Processes, and Application*, Series: *Physics of Atoms and Molecules*, (Kluwer, New York, 1999) pp. 213–224.
7. M. Reiher, B. Hess, in *Modern Methods and Algorithms of Quantum Chemistry,* ed. by J. Grotendorst, John von Neumann Institute for Computing, Julich, NIC Series, vol 3, (2000) pp. 479–505.
8. H.M. Quiney, in *Relativistic Quantum Mechanics of Atoms and Molecules. New Trends in Quantum Systems in Chemistry and Physics*, Series: *Pro-*

gress in Theoretical Chemistry and Physics, vol 6 (Springer, Berlin, 2002) pp. 135–173.

9. S. Wilson, Journ. of Mol. Str.: Theochem. **547**, 279–291 (2001)
10. I.P. Grant, H.M. Quiney, Int. J. Quantum Chem. **80**, 283 (2000)
11. *Advanced Topics in Theoretical Chemical Physics,* Series: *Progress in Theoretical Chemistry and Physics*, vol. 12, ed. by J. Maruani, R. Lefebvre, E. Brändas (Springer, Berlin, 2004)
12. *H.Jensen, T.Saue, L.Visscher with contr. by V.Bakken, E.Eliav, T. Enevoldsen, T.Fleig, O.Fossgaard, T.Helgaker, J.Laerdahl, C.Larsen, P. Norman, J.Olsen, M.Pernpointner, J.Pedersen, K.Ruud, P.Salek, J. van Stralen, J.Thyssen,O. Visser, T.Winther, DIRAC Code, a relativistic ab initio electronic structure program, Release DIRAC4.0.-2004; (*http://dirac.chem.sdu.dk*).*
13. *W.*Martin, *NIST Spectra Database, version 2.0*, NIST, Washington,2004; *(http:// physics.nist.gov.asd).*
14. *C. Moore, NBS Spectra Database*, NBS, Washington, 1987.
15. A.V. Glushkov, S.V. Ambrosov, A.V. Loboda, E.P. Gurnitskaya, O.Yu. Khetselius, in *Recent Advances in Theoretical Physics and Chemistry Systems*, Series: *Progress in Theoretical Chemistry and Physics*, vol. 15, ed. by J.-P. Julien, J. Maruani, D. Mayou, S. Wilson, G. Delgado-Barrio (Springer, Berlin, 2006), pp. 285-300.
16. A.V. Glushkov, O.Yu. Khetselius, E.P. Gurnitskaya, A.V. Loboda, T.A. Florko, D.E. Sukharev, L. Lovett, in *Frontiers in Quantum Systems in Chemistry and Physics*, Series: *Progress in Theoretical Chemistry and Physics*, vol. 18, ed. by S. Wilson, P.J. Grout., J. Maruani, G. Delgado-Barrio, P. Piecuch (Springer, Berlin, 2008), p.501-522
17. A.V. Glushkov, O.Yu. Khetselius, L. Lovett, L., in: *Advances in the Theory of Atomic and Molecular Systems Dynamics, Spectroscopy, Clusters, and Nanostructures*. Series: *Progress in Theoretical Chemistry and Physics*, vol. 20, ed. by P.Piecuch, J. Maruani, G. Delgado-Barrio, S. Wilson (Springer, Berlin, 2010), pp.125-172.
18. A.V. Glushkov, S.V. Ambrosov, A.V. Loboda, Yu.G. Chernyakova, O.Yu. Khetselius, A.A. Svinarenko, Nucl. Phys. A **734**S, 21 (2004)
19. A.V.Glushkov, S.V.Malinovskaya, O.Yu. Khetselius, D.E.Sukharev,

A.V.Loboda, L.Lovett, Int. Journ. of Quant.Chem. **109**, 1417 (2009).

20. *Photonic, Electronic and Atomic Collisions*, ed. by F. Aumar and H. Winter (World Scientific, Singapore, 1997), pp.1-650.

21. M. Hehenberger, H. McIntosh, E. Brändas, Phys. Rev. A **10**, 1494 (1974).
22. E.Brändas, P. Floelich, Phys. Rev.A **16**, 2207 (1977).

23. J.C. Slater, *The Consistent Field Method for Molecules and Solids: Quantum Theory of Molecules and Solids*, vol. 4 (McGraw-Hill, New York, 1974).
24. S. Wilson, in *Recent Advances in Theoretical Physics and Chemistry Systems*, Series: *Progress in Theoretical Chemistry and Physics*, vol. 16, ed. by J. Maruani, S. Lahmar, S. Wilson, G. Delgado-Barrio (Springer, Berlin, 2007), p. 11-80.
25. S. Wilson, *Handbook on Molecular Physics and Quantum Chemistry* (Wiley, Chichester, 2003).
26. I. Theophilou, S. Thanos, A. Theophilou, J. Chem. Phys. **127**, 234103 (2007).
27. D.J. Dean, M. Hjorth-Jensen, K. Kowalski, P. Piecuch, M. Wloch, in *Condensed Matter Theories*, ed. by J.W. Clark, R.M. Panoff, H. Li (Nova Sci. Publishers, 2006).
28. P. Piecuch, M. Wloch, J.R. Gour, D.J. Dean, M. Hjorth-Jensen, T. Papenbrock, in *Nuclei and Mesoscopic Physics: Workshop on Nuclei and Mesoscopic Physics* WNMP 2004, AIP Conference Proceedings, vol. 995, ed. by V. Zelevinsky (American Institute of Physics, Melville, NY, 2005), p. 28.
29. W. Kohn, L.J. Sham, Phys. Rev. A **140**, 1133 (1964).
30. P. Hohenberg, W. Kohn, Phys. Rev. B **136**, 864 (1964).
31. E.G. Gross, W. Kohn, *Exchange-Correlation Functionals in Density Functional Theory* (Plenum, New York, 2005).
32. *The Fundamentals of Electron Density, Density Matrix and Density Functional Theory in Atoms, Molecules and the Solid State*, Series: *Progress in Theoretical Chemistry and Physics*, vol. 14, eds. N. Gidopoulos and S. Wilson (Springer, Berlin, 2004), p.1.

33. R.M. Dreizler, Phys. Scripta T **46**, 167 (1993).
34. E.Clementi, C.Roetti, Atom. Data Nucl. Data Tables. **14**, 177 (1974).
35. C.Froese Fischer, G.Tachiev, Atom. Data Nucl. Data Tables. 87, 1 (2004).
36. C.Froese Fischer, G.Tachiev, A. Irimia, GAtom. Data Nucl. Data Tables. 92, 607 (2006).
37. E.Luc-Koenig, A. Lyras, J.-M. Lecomte, M. Aymar, J.Phys. B: At. Mol. Opt. Phys. **30**, 5213 (1997).
38. M.A.Klapish, Comp.Phys.Commun. **2**, 239 (1971).
39. C.Laughlin, G.A. Victor, Adv. Atom. Mol. Phys. **25,** 163 (1988).

40. P.Durand, J.Malrieu, *Ab initio quantum chemistry methods* Wiley, New York, 1987).
41. J.Bieron, C.Froese-Fischer, S.Fritzsche, K. Pachucki, J.Phys.B:At.Mol.Opt.Phys. **37**, L305 (2004).
42. K.N. Koshelev, L.N. Labzowsky, I.I. Tupitsyn, J. Phys. B **37**, 843 (2004)
43. J. Bieron, P. Pyykkö, P. Jonsson, Phys. Rev. A **71**, 012502 (2005).
44. J. Bieron, P. Pyykkő, Phys. Rev. A **71**, 032502 (2005).
45. P. Mohr, Atom. Data Nucl. Data Tabl**. 24**, 453 (1993); Phys. Scripta T **46**, 44 (1993).
46. M.P. Das, M.V. Ramana, A.K. Rajagopal, Phys. Rev. **22**, 9 (1980).
47. K. Cheng, Y. Kim, J. Desclaux, Atom. Data Nucl. Data Tabl. **24**, 11 (1979).
48. G. Drake, Phys. Scripta T **46**, 116 (1993).
49. H.M. Quiney, I.P. Grant, Phys. Scripta T **46**, 132 (1993).
50. G. Gould, Phys. Scripta T**46**, 61 (1993).
51. S. Blundell, Phys. Scripta T **46,** 144 (1993).
52. C.Froese-Fischer, Phys.Rev.A**39**, 963 (1989).
53. A.Weiss, J.Quant.Spectr. Radiat.Transf. **18**, 481 (1977).
54. W.R.Johnson, C.D.Lin, K.T.Cheng, Phys.Scr. **21**, 409 (1980).
55. W.R.Johnson, J.Sapistein, S.Blundell, Phys.Rev.A**37**, 307 (1988).
56. W. Johnson, J. Sapirstein, S. Blundell, Phys. Scripta 46, 184 (1993).
57. P. Indelicato, J.P. Desclaux, Phys. Scripta T **46**, 110 (1993)
58. V. Dzuba, V. Flambaum, P. Silvestrov, O. Sushkov, Phys. Rev. A **44**, 2828 (1991).

59. H. Persson, I. Lindgren, S. Salomonson, Phys. Rev. Lett. **76**, 204 (1996).
60. S.N. Tiwary, Rivista del Nuovo Cimento **18**, 1 (1995).
61. J. Bieron, C. Froese-Fisher, S. Fritzsche, K. Pachucki, J. Phys. B: At. Mol. Opt. Phys. **37**, L305 (2004).
62. U. Safranova, T. Cowan, M. Safranova, J. Phys. B: At. Mol. Phys. **38**, 2741 (2005).
63. V. Dzuba, V. Flambaum, M.S. Safranova, Phys. Rev. A **73**, 022112 (2006)
64. W.R. Johnson, U.I. Safranova, M.S. Safranova, Phys. Rev. A.**67,** 062106 (2003).
65. U.I. Safranova, M.S. Safranova, W.R. Johnson, Phys. Rev. A **71**, 052506 (2005).
66. M.S.Safronova, W.R. Johnson, U.I. Safranova, T.Cowan, Phys.Rev.A.**74**, 022504 (2006).
67. U.I. Safranova, M.S. Safranova, S.M.Hamasha, P.Beiersdorfer, Atom. Data Nucl. Data Tabl. **92**, 47 (2006).
68. V. Yerokhin, A.N. Artemyev, V.M. Shabaev, Phys. Rev. A **75**, 062501 (2007)
69. B. Sahoo, G. Gopakumar, R. Chaudhuri, B. Das, H. Merlitz, U. Mahapatra, D. Mukherjee, Phys. Rev. A **68**, 040501 (2003)
70. J. Santos, F. Parenre, S. Boucard, P. Indelicato, J. Desclaux, Phys. Rev. A **71**, 032501 (2005)
71. A. Derevianko, S.G. Porsev, Phys. Rev. A **71**, 032509 (2005)
72. O.Yu. Khetselius, Phys. Scripta. T.**135**, 014023 (2008).
73. O.Yu. Khetselius, Int. Journ.Quant.Chem. **109**, 3330 (2009).
74. M.J.Jamieson, G.W.F.Drake, A.Dalgarno, Phys.Rev. A **51,** 3358 (1995).
75. L.Curtis, Phys.Rev.A**35**, 2089 (1987).
76. B.Saha, S.Fritzsche, J.Phys. B: At. Mol. Opt. Phys.**38**, 1161 (2005).
77. A.Hibbert, J.E.Hansen// J.Phys. B: At. Mol. Opt. Phys. **27**, 3325 (1994).
78. M.D.Kunisz, Acta Phys.Polon.A **62**, 285 (1982).
79. M. Grance, Atomic Data. **5**, 185 (1973).
80. W.C.Jupen, B.Denne, I.Martinson, Phys.Scripta. **41,** 669 (1990).
81. J.Migdalek, Can.J.Phys. **54,** 130 (1976).
82. V.N. Ostrovsky, S.A.Sheynerman, Opt. Spectr. (USSR) **67**, 16 (1989).
83. S.A.Kotochigova, Opt.Spectr. (USSR) **55**, 422 (1983).

84. S.L.Mandelstam, E.V.Aglitsky, P.S.Antsiferov, A.M.Panin, Canad. J.Phys. 62, 1923 (1984).
85. E.K.Anderson, E.M.Anderson, Opt.Spectr. (USSR). **54,** 955 (1983).
86. P. Quinet, C. Argante, V. Fivet, C. Terranova1, A. V. Yushchenko, É. Biémont, Astrophys. Astron. **474**, 307 (2007).
87. É. Biémont, V. Fivet, P. Quinet, J.Phys. B: At. Mol. Opt. Phys 37, 4193 (2004).
88. Bieron, J., Froese Fischer, C., Fritzche, S., & Pachucki, K. J.Phys. B: At. Mol. Opt. Phys 37, L305 (2004).
89. L.N. Labzovsky, JETP, **57**, 663 (1969); M.A.Braun, Yu.Yu.Dmitriev, L.N.Labzovsky, JETP. **57,** 2189 (1969).
90. L.N.Ivanov, E.P.Ivanova, Atom.Data Nucl. Data Tabl. **24**, 95 (1979).
91. L.N.Ivanov, M.N.Driker, Opt.Spectr. (USSR) **49**, 209 (1980).
92. M.N.Driker, E.P.Ivanova, L.N. Ivanov, A.F.Shestakov, J.Quant.Spectr. Rad.Transf. **28, 531 (**1982).

93. E.P. Ivanova, L.N. Ivanov, A.V. Glushkov, A. Kramida, Phys. Scripta **32**, 512 (1985).
94. E.P. Ivanova, A.V. Glushkov, J. Quant. Spectr. Rad. Transfer. **36**, 127 (1986).
95. L.N. Ivanov, V.S. Letokhov, JETP **68**, 748 (1975); JETP **71**, 19 (1976).
96. L.N. Ivanov, V.S. Letokhov, Com.Mod.Phys.D.:At.Mol.Phys. **4**, 169 (1985).
97. A.V. Glushkov, E.P. Ivanova, in: *Spectroscopy of multicharged ions*, ed. U.I.Safronova (Nauka, Moscow, 1986), pp.5-195.
98. A.V. Glushkov, S.V.Malinovskaya, Opt. Spectr. (USSR) **62**, 966 (1987); **62**, 1212 (1987).
99. A.V. Glushkov, Opt. Spectr. (USSR) **64,** 446 (1988); **65,** 1175 (1988).
100. A.V. Glushkov, S.V.Malinovskaya, in: *Many-body effects in atoms*, ed. U.I.Safronova (Nauka, Moscow, 1988), pp.73-189.
101. E.Vidolova-Angelova, L.N.Ivanov, E.P.Ivanova, V.S.Letokhov, Izv. AN USSR. Ser. Phys. **45**, 2300 (1981).
102. G.I. Bekov, E.Vidolova-Angelova, L.N.Ivanov, E.P.Ivanova, V.S.Letokhov, V.I.Mishin, JETP. **80,** 866 (1981).

103. E.Vidolova-Angelova, L.N.Ivanov, E.P.Ivanova, Opt. Spectr. (USSR). **50,** 243 (1981); Opt. Spectr. (USSR). **54**, 590 (1983).
104. E.Vidolova-Angelova, L.N.Ivanov, E.P.Ivanova, D.A.Angelov, J.Phys.B: At. Mol. Opt. Phys.**19,**-2053 (1986).
105. E.Vidolova-Angelova, L.N.Ivanov, J. Phys.B:At.Mol.Opt.Phys. **21**, 3877 (1988).
106. E.Vidolova-Angelova, L.N.Ivanov, J. Phys.B:At.Mol.Opt.Phys. **24**, 4147 (1991).
107. A.V. Glushkov, Sov. Phys. J. **40,** 34 (1991); **41** (N9)**,** 3 (1992).
108. L.N. Ivanov, E.P. Ivanova, JETP. **110**, 483 (1996)
109. E.P. Ivanova, L.N. Ivanov, E.V. Aglitsky, Phys. Rep. **166**, 315 (1988).
110. L.N. Ivanov, E.P. Ivanova, L. Knight, Phys. Rev. A **48,** 4365 (1993)
111. K.N. Koshelev, L.N. Ivanov, Phys. Rev. A **42**, 5784 (1990)
112. E.P. Ivanova, A.V.Gulov, Atom.Data.Nucl.Data.Tabl. **49**, 1 (1991).
113. E.P.Ivanova,A.Gogava, in: *Spectroscopy of autoionization states for atoms and ions*, ed. U.I.Safronova (Nauka, Moscow, 1988), pp.212-256.
114. E.P. Ivanova, I.P. Grant, J. Phys.B:At.Mol.Opt.Phys. **31**, 2871 (1998).
115. E.P. Ivanova, N.A. Zinoviev, Quant. Electronics **29**, 484 (1999).
116. E.P.Ivanova, N.A.Zinoviev, Phys. Lett.A. ,Vol.**274**, 239 (2001).
117. A.V. Glushkov, L.N. Ivanov, E.P Ivanova, *Autoionization Phenomena in Atoms*, (Moscow University Press, Moscow, 1986) pp.152-164.
118. A.V. Glushkov, J. Appl. Spectr. **52,** 297 (1990); **56,** 13 (1992); **56,** 482 (1992).
119. A.V. Glushkov, Opt. Spectr. (USSR). **66**, 31 (1989); **66**, 1180 (1989); **70**, 952 (1991).
120. A.V. Glushkov, Opt. Spectr. (USSR) **71**, 395 (1991); **72,** 55 (1992); **72,** 542 (1992).
121. A.V. Glushkov, JETP Lett. 55, 97 (1992).
122. A.V. Glushkov, Rus. J. Struct. Chem. **31**, 9 (1990); **32**, 11 (1992); **34**, 3 (1993).
123. A.V. Glushkov, Rus. J. Phys. Chem. **66**, 589 (1992); **66**, 1259 (1992).
124. A.V. Glushkov, L.N. Ivanov, Preprint of Institute for Spectroscopy of USSR Academy of Sciences (ISAN), AS N1 (ISAN, Moscow-Troitsk, 1992), pp.1-16.

125. A.V. Glushkov, L.N. Ivanov, Preprint of Institute for Spectroscopy of USSR Academy of Sciences (ISAN), AS N2 (ISAN, Moscow-Troitsk, 1992), pp.1-10.
126. A.V. Glushkov, L.N. Ivanov, Preprint of Institute for Spectroscopy of USSR Academy of Sciences (ISAN), AS N3 (ISAN, Moscow-Troitsk, 1992), pp.1-12.
127. A.V. Glushkov, L.N. Ivanov, V.S.Letokhov, Preprint of Institute for Spectroscopy of e USSR Academy of Sciences (ISAN), AS N4 (ISAN, Moscow-Troitsk, 1992), pp.1-16.
128. A.V. Glushkov, L.N. Ivanov, Phys. Lett. A **170**, 33 (1992);
129. A.V.Glushkov, S.V.Malinovskaya, Sov. Phys. J. **41 (**N11), 3 (1992).
130. A.V. Glushkov, L.N. Ivanov, Atomic Spectroscopy (Inst. Chem.Phys. AS, Chernogolovka, 1992), p.113.
131. A.V. Glushkov, L.N. Ivanov, J. Phys. B: At. Mol. Opt. Phys. **26,** L379 (1993)
132. A.V.Glushkov, S.V.Malinovskaya, S.V.Ambrosov, in: *Atomic Spectra and Oscillator Strengths for Astrophysical and Laboratory Plasmas* (Publ.de l'Observatoire de Paris, Meudon, 1996), pp.96-101.
133. A.V. Glushkov, in *Low Energy Antiproton Physics:* Eighth International Conference on Low Energy Antiproton Physics (LEAP '05), AIP Conference Proceedings, vol. 796, ed. by D. Grzonka, R. Czyzykiewicz, W. Oelert, T. Rozek, P. Winter (American Institute of Physics, Melville, NY, 2005), p. 206-215.
134. A.V. Glushkov, O.Yu. Khetselius, A.V. Loboda, E.P. Gurnitskaya, in *Meson-Nucleon Physics and the Structure of the Nucleon*, ed. by S. Krewald, H. Machner (IKP, Juelich, Germany), SLAC eConf C070910 (Menlo Park, CA, USA) **2**, 186 (2007); A.V.Glushkov, ibid. **2**, 111 (2007)
135. A.V. Glushkov, S.V. Malinovskaya, L.A.Vitavetskaya, Yu.V. Dubrovskaya, O.Yu. Khetselius, in: *Recent Advances in Theoretical Physics and Chemistry Systems*, Series: *Progress in Theoretical Chemistry and Physics*, vol. 15, ed. by J.-P. Julien, J. Maruani, D. Mayou, S. Wilson, G. Delgado-Barrio (Springer, Berlin, 2006), pp. 301-318.
136. A.V. Glushkov, S.V. Malinovskaya, Rus. J. Phys. Chem. **62**, 100 (1988).
137. A.V. Glushkov, S.V. Malinovskaya, Rus. J. Phys. Chem.**62**, 2970 (1988).

138. A.V. Glushkov, S.V. Malinovskaya, in *New Projects and New Lines of Research in Nuclear Physics*, ed. by G. Fazio, F. Hanappe (World Scientific, Singapore, 2003), pp.242-264.
139. A.V.Glushkov, O.Yu. Khetselius, in: *Nuclear Physics in Astrophysics* NPA-III (Dresden, Germany, 2007), p. 95; J. Phys. G., to be published.
140. A.V. Glushkov, S. Malinovskaya, A. Loboda, G. Prepelitsa, J. Phys.: Conf. Ser. **35**, 420 (2006)
141. A.V. Glushkov, S. Malinovskaya, E. Gurnitskaya, O. Khetselius, J. Phys.: Conf. Ser. **35**, 426 (2006)
142. A.V. Glushkov, S.V. Malinovskaya, A.V. Loboda, E.P. Gurnitskaya, D.A. Korchevsky, J. Phys.: Conf. Ser. **11**, 188 (2005)
143. A. Glushkov, S. Malinovskaya, G. Prepelitsa, V. Ignatenko, J. Phys.: Conf. Ser. **11**, 199 (2004)
144. A.V. Glushkov, I.T. Makarov, E. Nikiforova, M.I. Pravdin, I.E. Sleptsov, Astroparticle Physics **4**, 15 (1995)
145. A.V. Glushkov, L.G. Dedenko, M.I. Pravdin, I.E. Sleptsov, JETP **99,** 123 (2004).
146. A.V. Glushkov, S.V. Malinovskaya, Yu.G. Chernyakova, A.A. Svinarenko, Int. J. Quantum Chem. **99**, 889 (2004).
147. A.V. Glushkov, S.V. Malinovskaya, Int. J. Quantum Chem. 104, 496 (2005).
148. A. Glushkov, S. Malinvoskaya, O. Khetselius, Eur. Phys. J. ST **160**, 195 (2008).
149. A. Glushkov, S. Malinvoskaya, O. Khetselius, Mol. Phys. **106**, 1257 (2008).

150. A.V. Glushkov, O.Yu. Khetselius, S.V. Malinovskaya, in *Frontiers in Quantum Systems in Chemistry and Physics*, Series: *Progress in Theoretical Chemistry and Physics* , vol. 18, ed. by S.Wilson, P.J.Grout, J. Maruani, G. Delgado-Barrio, P. Piecuch (Springer, Berlin, 2008), pp. 523-540.
151. A.V. Glushkov, J. Appl.Spectr. (Springer) **74**, 305 (2007).
152. A.V. Glushkov, Sensor Electr. Microsyst. Techn. **3**, 21 (2006); **4**, 11 (2007); **5**, 41 (2008).

153. A.V. Glushkov, S.V. Ambrosov, A.V. Ignatenko, D.A. Korchevsky, Int. J. Quantum Chem. **99**, 936 (2004).
154. A.V. Glushkov, S.V. Malinovskaya, I.M. Shpinareva, V.P. Kozlovskaya, V.I. Gura, Int. J. Quantum Chem. **104**, 512 (2005).
155. Glushkov, A.V., Ambrosov, S.V., Loboda, A.V., Gurnitskaya, E.P., Prepelitsa, G.P. Int. J. Quantum Chem. **104**, 562 (2005).
156. A.V. Glushkov, A.V.Loboda, E.P. Gurnitskaya, A.A.Svinarenko, Phys. Scripta T **134**, 137740 (2009).
157. A.V. Glushkov, V.D. Rusov, S.V. Ambrosov, A.V. Loboda, in *New Projects and New Lines of Research in Nuclear Physics*, ed. by G. Fazio and F. Hanappe (World Scientific, Singapore, 2003), p. 126-142.
158. A.V. Glushkov, O.Yu. Khetselius, A.V.Loboda, A.A.Svinarenko, in *Frontiers in Quantum Systems in Chemistry and Physics*, Series: *Progress in Theoretical Chemistry and Physics*, vol. 18, ed. by S. Wilson, P.J. Grout., J. Maruani, G. Delgado-Barrio, P. Piecuch (Springer, Berlin, 2008), pp.541-588.
159. A.V. Glushkov, O.Yu. Khetselius, S.V.Malinovskaya, in *Frontiers in Quantum Systems in Chemistry and Physics*, Series: *Progress in Theoretical Chemistry and Physics*, vol. 18, ed. by S. Wilson, P.J. Grout., J. Maruani, G. Delgado-Barrio, P. Piecuch (Springer, Berlin, 2008), pp.523-540.
160. A.V. Glushkov, Spectral Line Shapes (AIP) **1092**, 258 (2010).
161. V.V.Tolmachev, Adv. Quant. Chem. **4**, 331 (1969).
162. V.S.Letokhov, Preprint of Physical Institute of the USSR Academy of Sciences (FIAN), N1-69 (FIAN. Moscow, 1969), pp.1-72.
163. V.S. Letokhov, Phys. Lett. A **46**, 257 (1974).
164. V.S. Letokhov, Laser Specktroskopie (Akad.-Verlag, Berlin, 1977).
165. V.I.Goldansky, V.S. Letokhov, Sov. Phys. JETP. **67**,513 (1974).
166. G.G.Baldwin, J.C.Salem, V.I.Goldansky, Rev.Mod.Phys. **53**, 687 (1981).
167. N.G.Basov, V.S.Letokhov, Sov.Phys.-Uspekhi. **11**, 855 (1969).
168. V.S. Letokhov, Science. **180** (N4085), 451 (1973).
169. V.S. Letokhov, L.N.Ivanov, Quantum Electronics (USSR) **2 (**N3), 585 (1975).
170. V.S. Letokhov, V.G.Minogin, B.D.Pavlik, Optics Comm. **19**, 72 (1976).
171. V.S. Letokhov, C.B.Moore, *Chemical and Biochemical Applications of*

Lasers. (Acad.Press, New York, 1977), pp.1-670.
172. V.S. Letokhov, Nature, N**277**, 605 (22 February 1979).
173. V.S. Letokhov, in: *Apllication of Lasers in Atomic, Molecular and Nuclear Physics*, ed. by A.M.Prokhorov and V.S.Letokhov (Nauka, Moscow, 1979), pp.412-455.
174. V.S. Letokhov, V.I.Balykin, V.I.Mishin, G.I.Bekov, Sov.Phys.-Uspekhi. **132** (N10) 79 (1980).
175. V.S. Letokhov, *Nonlinear Selective Photo-processes in atoms and molecules* (Nauka, Moscow, 1983), pp.1-408.
176. V.S. Letokhov, V.G. Minogin, Sov.Phys.-Uspekhi. **147** (N9), 79 (1985).
177. V.S. Letokhov, Sov.Phys.-Uspekhi. **29**, 70 (1986); **41**, 523 (1998); **42**, 241 (1999).
178. V.S. Letokhov, V.I.Balykin, Sov.Phys.-Uspekhi. **33**, 79 (1990); Phys. Rev. A.**64**, 063410 (2001).
179. V.S. Letokhov, L.N.Ivanov, A.V.Glushkov, Preprint of Institute for Spectroscopy of USSR Academy of Sciences (ISAN), AS N5 (ISAN, Moscow-Troitsk, 1992), p.1-18.
180. N.G.Basov, E. Belenov, V.A.Isakov, E.A.Markin, Sov.Phys.-Uspekhi. **121**, 427 (1977).
181. V.S.Lisitsa, Sov.Phys.-Uspekhi. **153**, 379 (1977).
182. A.M.Prokhorov, N.V.Karlov, B.B.Krynetsky, V.A.Mishin, Sov.Phys.-Uspekhi. **137**, 593 (1979).
183. P.A. Bokhan, V.V.Buchanov, N.V.Fateev, M.M.Kalugin, M.A.Kazaryan, A.M.Prokhorov, D.E.Zakrevskii, *Laser Isotope Separation in Atomic Vapor* (Wiley-VCH, Berlin, 2006).
184. V.V.Buchanov, M.A.Kazaryan, M.Kalugin, A.M.Prokhorov, *Laser separation of Silicon Isotopes by the AVLIS Technology*, Series: *Atomic and Molecular Pulsed Lasers* (SO RAN, Tomsk, 2001).
185. W.Stoll, *Present Status of industrial Isotope separation by laser technology*, Series: *Atomic and Molecular Pulsed Lasers* (SO RAN, Tomsk, 2001).
186. F.J. Duarte, *Tunable Laser Optics* (Elsevier Academic, New York, 2003).
187. F.J. Duarte, Australian Physics. **47**, 38 (2010).
188. G.S., Janes, H.K., Forsen, R.H. Levy, The Exxon/Avco Program in Laser Enrichment: Uranium Enrichment; Research Report, N422 (Avco Everett

Res. Lab., 1975).
189. S.Singh, K.Dasgupta, S.Kumar, K.Manohar, L.Nair, O. Chatterjee, Opt. Eng**. 33**, 1894 (1994).
190. R.W. Solarz, C.A.May, L.R.Carlson, E.F.Worden, S.A.Johnson, J.A.Paisner, L.J. Radziemski, Phys.Rev.A. **14**, 1129 (1976).
191. A.V. Glushkov, *Atom in an electromagnetic field* (KNT, Kiev, 2005), 450p.

CHAPTER 2. RELATIVISTIC ENERGY APPROACH IN MATHEMATICAL PHYSICS OF RADIATIVE AND AUTOIONIZATION PROCESSES IN HEAVY FINITE FERMI-SYSTEMS: APPLICATIONS

2.1 Radiative transition probabilities and oscillator strengths for transitions in spectra of some heavy atoms and ions

We have presented (Chapter 1) the generalized energy approach (Gell-Mann and Low S-matrix formalism) to relativistic calculation of the radiative and autoionization characteristics for multielectron atoms and ions. Here the results of relativistic calculation of the radiative transitions probabilities, oscillators strengths, autoionization widths are (some part firstly) presented for a number of heavy atoms and multicharged ions and discussed from point of view of the correct accounting for the relativistic and exchange-correlation effects. The data on autoionization processes in heavy atoms and ions can be used for carrying out the optimal schemes of the laser photoionization isotope separation method.

Here we present the calculation results for the probabilities and oscillator strengths of the radiative transitions in spectra of the heavy atoms and ions of Hg^+, Eu, Yb. Some additional details can be found in Refs. [13,14,80-84,101-103]. Especial interest to studying these transitions is explained by importance of the corresponding data for laser effect research. The collision of atoms of the Mendeleyev table second raw with ions of helium (other inert gases) leads to creating ions in the excited states that it is important for creating the inverse populations and laser effect. Available in the literature data about radiative characteristics are definitely insufficient. An account of the relativistic and correlation effects has a critical role in the cited systems as the studied transitions occur in the external shells in a strong field of atom with large nuclear charge (Z=80). The corresponding Hg^+ states can be treated within the QED PT formalism as one- and three-QP states of electrons (6s) and vacancy ($5d^{-1}$) above the core of the closed electron shells $5d^{10}6s^2$. The interaction QP-core is described by the potentials (7),(13), which imitate the DF potential. The polarization interaction of the QPs through the polarizable core is described by the two-particle effective potential [93]. In table 2.1-2.3 we present the energies, electric E1

($5d^{10}7p(P_{1/2},P_{3/2})$-$5d^{10}6s(S_{1/2})$, $5d^{10}7p(P_{1/2},P_{3/2})$-$5d^{10}7s(S_{1/2})$) and E2 ($5d^{9}6s^{2}(D_{5/2},D_{3/2})$- $5d^{10}6s$ $(S_{1/2})$) probabilities of the corresponding transitions in spectra Hg^{+}, which are calculated within the energy approach and QED PT (from refs.[13,14,83,84,120,124]).

Table 2.1

The energies of the $5d^{9}6s^{2}(D_{5/2},D_{3/2})$- $5d^{10}6s$ $(S_{1/2})$, $5d^{10}7p(P_{1/2},P_{3/2})$-$5d^{10}6s(S_{1/2})$, $5d^{10}7p(P_{1/2},P_{3/2})$-$5d^{10}7s(S_{1/2})$, $5d^{9}6s^{2}(D_{5/2},D_{3/2})$- $5d^{10}6s$ $(S_{1/2})$ transitions in Hg^{+} (Ry): theoretical data – HF, DF, QED PT; experimental data - Moore (NBS, Washington).

Method	E_{6s}	$7P_{1/2}$-$6S_{1/2}$	$7P_{3/2}$-$6S_{1/2}$	$7P_{1/2}$-$7S_{1/2}$	$7P_{3/2}$-$7S_{1/2}$	$D_{3/2}$-$S_{1/2}$	$D_{5/2}$-$S_{1/2}$
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
QED PT	-1.377	0.986	1.019	0.114	0.147	0.462	0.325
Exp..	-1.378	0.987	1.020	0.115	0.148	0.461	0.324

Table 2.2

Probabilities of the 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-Fock data, DF (E_{exp}) – DF data with using the experimental transitions energies; QED PT– our method; exp. - Moore (NBS, Washington)

Method	$7P_{3/2}$-$6S_{1/2}$	$7P_{1/2}$-$6S_{1/2}$	$7P_{3/2}$-$7S_{1/2}$	$7P_{1/2}$-$7S_{1/2}$
HF	$4.75\cdot10^{6}$	$4.75\cdot10^{6}$	$3.65\cdot10^{7}$	$3.65\cdot10^{7}$
DF	$8.45\cdot10^{7}$	$1.67\cdot10^{7}$	$6.89\cdot10^{7}$	$4.71\cdot10^{7}$
DF (E_{exp})	$1.17\cdot10^{8}$	$2.04\cdot10^{7}$	$1.10\cdot10^{8}$	$5.52\cdot10^{7}$
QED PT	$1.49\cdot10^{8}$	$2.31\cdot10^{7}$	$1.41\cdot10^{8}$	$6.33\cdot10^{7}$
Exp.	$1.53\cdot10^{8}$	$2.35\cdot10^{7}$	$1.44\cdot10^{8}$	$6.37\cdot10^{7}$

Table 2.3

The E2 probabilities of the $5d^96s^2(D_{5/2},D_{3/2})$- $5d^{10}6s$ $(S_{1/2})$ transition in Hg^+ (in s^{-1}): HF- Hartree-Fock data, DF – Dirac-Fock data, DF (E_{exp}) – DF data with using the experimental transitions energies; QED PT– our method; exp. - Moore (NBS, Washington)

Method	$D_{3/2}$- $S_{1/2}$	$D_{5/2}$- $S_{1/2}$
HF	1360	1360
DF	257.0	77.4
DF (E_{exp})	63.9	13.3
QED PT	54.53(0,2%)	11.84 (0,2%)
Exp.	53.5±2.0	11.6±0.4

For comparison we listed the theoretical Hartree-Fock (HF), Dirac-Fock (DF) and DF (with fitting to experimental transition energies) values by Ostrovsky-Sheynerman and experimental data by Moore (NBS, Washington) (from refs.[13,14,83,84,120]) in the tables 2.1-2.3. The standard HF and DF approaches in the single-configuration approximations don't allow to receive the accurate results.

Using the empirical transition energies significantly improve the theoretical results as it means in fact account of the very important interelectron correlations effects. In the QED PT formalism the corresponding exchange-correlation effects (the polarization interaction of the QPS, mutual screening and anti-screening corrections etc) are taken into account more accurately.

Let us note that the core polarization correction to the transition probabilities is of a great importance as it changes the probability value on 15-40%. It should be also noted that the gauge –noninvariant contribution to radiation width is very small (0,2%; see table 2.2 in the line "QED PT") that means equivalence of the calculation results in the standard amplitude approach with using the length and velocity forms for transition operator.

From other side this is an evidence of the successful choice of the PT zeroth approximation and accurate account of the multi-particle correlation effects.

Further in table 2.4 we listed the theoretical energies of some transitions in spectra of atoms EuI.

In table 2.5 we present our results of calculating (column F) the oscillator strengths of the electric dipole transitions (table 2.4). Here the optimized DF scheme within QED PT has been used.

For comparison there are also listed the results of calculations within the Coulomb approximation method (columns A,B,C are corresponding to the gauges of the photon propagator: Coulomb, Babushkin, Lamdau), multiconfiguration DF method (D), experimental data (E1,E2) (from Refs. [13,79,120]).

Table 2.4

Theoretical transitions energies in EuI (from Refs. [13,79,120]).

N	Transition	Wavelength (in Å)
1	$4f^7(^8S)6s^2\ ^8S_{7/2} \rightarrow 4f^7(^8S)6s6p\ ^8P_{5/2}$	4661,88
	$4f^7(^8S)6s^2\ ^8S_{7/2} \rightarrow 4f^7(^8S)6s6p\ ^8P_{7/2}$	4627,22
3	$4f^7(^8S)6s^2\ ^8S_{7/2} \rightarrow 4f^7(^8S)6s6p\ ^8P_{9/2}$	4592,03
4	$4f^7(^8S)6s^2\ ^8S_{7/2} \rightarrow 4f^7(^8S)6s7p\ ^8P_{5/2}$	2743,28
5	$4f^7(^8S)6s^2\ ^8S_{7/2} \rightarrow 4f^7(^8S)6s7p\ ^8P_{9/2}$	2738,57
6	$4f^7(^8S)6s^2\ ^8S_{7/2} \rightarrow 4f^7(^8S)6s7p\ ^8P_{7/2}$	2731,37
7	$4f^7(^8S)6s^2\ ^8S_{7/2} \rightarrow 4f^7(^8S)6s8p\ ^8P_{9/2}$	2471,14
8	$4f^7(^8S)6s^2\ ^8S_{7/2} \rightarrow 4f^7(^8S)6s8p\ ^8P_{7/2}$	2461,78
9	$4f^7(^8S)6s^2\ ^8S_{7/2} \rightarrow 4f^7(^8S)6s8p\ ^8P_{5/2}$	2560,50

An analysis of the listed data shows that Athe Coulomb approximation results in different photon propagator gauges significantly differ from each other. In the QED energy approach this difference is not more that 0.1% for the Coulomb and Babushkin gauges. The contribution provided by the polarization and screening effects is very important for EuI (~35%). In table 2.6 we present theoretical and experimental data for the oscillator strengths of the ytterbium YbI low-lying states (from Refs.[101-104,124].

Table 2.5

The oscillator strengths of the E1 transitions in EuI (table 2.4): theoretical data - the Coulomb approximation method (columns A,B,C are corresponding to the gauges of the photon propagator: Coulomb, Babushkin, Lamdau), multiconfiguration DF method (column D)4 experimanmtal data (columns E1,E2).

N	A	B	C	D	E1	E2	F
1	0,205	0,264	0,469	0,280	0,433	0,49	0,478
2	0,272	0,350	0,622	0,374	0,588	0,59	0,591
3	0,342	0,439	0,781	0,540	0,740	0,74	0,740
4	0,0228	0,0293	0,052		0,012		0,015
5	0,0381				0,0024		0,028
6	0,0303				0,0047		0,022
7	0,0157				0,0015		0,0017
8	0,0098				0,0060		0,0063
9	0,0075				0,0045		0,0049

The presented data confirm a complexity of the studied object. The simple Coulomb approximation may hardly provide the necessary accuracy. All conclusions regarding the role of the correlation and gauge-noninvariant contributions are similar to previous case of the Eu atom.

Table 2.6

The oscillator strengths *f* of the ytterbium low-lying states transitions: Experiment – column E; theoretical data – the Coulomb approximation (CA; Coulomb gauge of the photon propagator); multiconfiguration DF method (column D); QED PT (column F).

Transition	λ (A)	*f, CA*	*f ,DF*	*f, QED PT*	f^{exp}
$4f^{14}6s^2\ ^1S_0$ - $4f^{14}6s6p\ ^1P_1$	3987,9	1,82	1,65	1,36[a]; 1,48[b]	1,2; 1,38; 1,12;
$4f^{14}6s^2\ ^1S_0$ – $4f^{14}6s7p\ ^1P_1$	2464,5	1,19	0,59	0,33[a]; 0,38[b]	0,22

Note: a – calculation with the optimized wave functions;

b – calculation with the non-optimized wave functions;

2.2 Radiative transition probabilities and oscillator strengths for transitions in spectra of Zn-like multicharged ions

Here we present the results of calculating probabilities of the magnetic dipole (M1) and electric quadrupole (E2) forbidden transitions for Zn-like multicharged ions (Z=32-92). In all calculations by QED PT it has been used the Ivanov-Ivanova model potential (7) with defining its parameter within above described an initio QED procedure. In fact this potential imitated the self-consistent Dirac-Fock potential. In table 2.7 we present the energy approach (EA; QED PT) oscillator strengths of the $4s^2(^1S_0)$- 4s4p ($^1P^0_1$) transition in the Zn-like multicharged ions, . For comparison we listed in this table the theoretical Hartree-Fock (HF), Dirac-Fock (DF), DF (with fitting to experimental transition energies) and model potential (MP) data [85,118,119].

Table 2.7

The experimental and theoretical values of the oscillator strengths of $4s^2(^1S_0)$- 4s4p ($^1P^0_1$) transition in the Zn-like ions.

Ion	Method	ΔE	f_L	f_V
Ga^+	DF	0.3351	1.89	1.98
	HF	0.2984	2.30	2.01
	DF (E_{exp})	0.3221	1.97	1.95
	MP	0.3076	1.68	1.73
	EA	0.3220	1.862	1.861
	Exp.	0.3221	1.85 ± 0.15	1.85 ± 0.15
As^{3+}	DF	0.5247	1.87	1.86
	EA	0.5142	1.575	1.574
	Exp.	0.5141	1.56 ± 0.23	1.56 ± 0.23
Gd^{34+}	DF	4.6685	1.12	1.10
	EA	4.6294	1.01	0.99
Yb^{40+}	DF	6.2564	1.12	1.10
	EA	5.1788	0.97	0.96
Au^{40+}	DF	9.6361	1.18	1.15
	EA	9,5256	1.02	1.01

Pb^{52+}	DF	11.1153	1.21	1.18
	EA	10.9715	1.13	1.13
U^{62+}	DF	17.8584	1.37	1.36
	HF	17.6087	1.41	1.47
	EA	17.6285	1.33	1.33
	Exp.	-	1.31 ± 0.05	1.31 ± 0.05

Analysis of the obtained data allows to make the following conclusions. Firstly, one can see that the energy approach (within QED PT) provides physically reasonable agreement with experiment. Secondly, we have checked that the results for oscillator strengths, obtained within our approach in different photon propagator gauges (Coulomb, Babushkin, Landau gauges) are practically equal, that is provided by using an effective QED energy procedure [4].

Thirdly, calculation has confirmed the great role of the interelectron correlation effects of the second and higher QED PT orders, namely, effects of the interelectron polarization interaction and mutual screening.

In table 2.8, 2.9 we present the M1 and E2 transitions probabilities in some Zn-like ions (our calculation) for transitions: (a) $4s4p\left(^3P_2^0\right)\to 4s4p\left(^3P_1^0\right)$; (b) $4s4p\left(^1P_1^0\right)\to 4s4p\left(^3P_2^0\right)$ [85,118,119].

Table 2.8

The probabilities of the forbidden M1 and E2 transitions in spectra of some ions of ZnI isoelectronic sequence (our data): (a) $4s4p\left(^3P_2^0\right)\to 4s4p\left(^3P_1^0\right)$ (b) $4s4p\left(^1P_1^0\right)\to 4s4p\left(^3P_2^0\right)$

Transition	M1 (a)	E2 (a)	M1 (b)	E2 (b)
Ga^+	0.009(1)	0.065(-3)	0.053(1)	0.39(0)
As^{3+}	0.051(1)	0.018(-2)	0.015(2)	0.022(1)
Gd^{34+}	0.081(6)	0.118(4)	0.047(6)	0.047(5)
Yb^{40+}	0.039(7)	0.399(5)	0.145(6)	0.026(6)
Au^{49+}	0.028(8)	0.104(6)	0.119(7)	0.029(7)
Pb^{52+}	0.047(8)	0.067(7)	0.215(7)	0.058(7)
U^{62+}	0.036(9)	0.059(8)	0.128(8)	0.101(8)

One could note that the M1 and E2 transition probabilities values are quicly increase with the growth of the nuclear charge of ion. Under transition from the Zn-like ion of As to the Zn-like uranium this growth is about 8 orders.

2.3 Radiative transition probabilities and autoionization widths for Ne-like multicharged ions

In tables 2.9 and 2.10 we present the values of probabilities of the radiation transitions between levels of the configurations $2s^2 2p^5 3s,3d,4s,4d$ and $2s2p^6 3p,4p$ in the Ne-like ions of the Ni XIX and Br XXVI (in s^{-1}; total angle

Table 2.9

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 Ni XIX (in s^{-1}; total angle moment J=1): a – the MCDF method; b- relativistic PT with the empirical zeroth approximation (RPTMP); c1 – our QED PT data (without correlation corrections); c2 – our QED PT data (with an account for the correlation corrections); exp.- experimental data (see text).

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

Table 2.10

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 – our QED PT data (without and with account for correlation corrections); exp.- experimental data [1-4,8-11,15,18,20,21].

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

moment J=1): a – the MCDF method; b- relativistic PT with the empirical zeroth approximation (RPTMP); c1 – our QED PT data (without correlation corrections); c2 – our QED PT data (with an account for the correlation corrections); exp.- experimental data [13-15, 84,93,94, 108-114].

Analysis of the obtained data allows to make the following conclusions. Firstly, one can see that the energy (QED PT) [117,128, 13-15] approach provides physically reasonable agreement with experiment and significantly more advantage able in comparison with standard Dirac-Fock method and little better than the relativistic PT with model zeroth approximation (RPTMP) method [93,94], though the last (RPTMP) results hitherto are considered as the most acceptable (see refs. [3,4,93,94,108-114]).

Secondly, we have checked that the results for the transition probabilities, obtained within our approach in different photon propagator gauges (Coulomb, Babushkin, Landau gauges) are practically equal, that is provided by using an effective QED energy procedure [128]. Thirdly, calculation has confirmed the great role of the inter electron correlation effects of the second and higher PT orders, namely, effects of the inter electron polarization interaction and mutual screening.

Further let us describe some calculated data for autoionization decay probabilities in the spectra of the multicharged ions on example of the Fe ion with one vacancy above the core $1s^2 2s^2 2p^6 3s^2 3p^6$. This ion of a great interest because of the high complexness of the spectrum and great actuality for astrophysical applications [3,4,86-88,93,94]. As the final state of the studied system after autoionization decay is the three-quasiparticle, the general number of the decay channels is sufficiently large, so we are limited only by summarized probability of the autoionization decay for the state $1s^2 2s^2 2p^6 3s^2 3p^6$ with definite quantum numbers of vacancies $n_1 l_1$ and $n_2 l_2$. The detailed information about total number of channels is presented in ref. [91,117]. In table 2.11 we present values of the "i-f" transitions energies, calculated by us within ab initio QED PT, and also results of calculations within the MCDF (by Klapish et al), relativistic PT (RPT) with empirical zeroth approximation (by Ivanov et al) and available experimental data (see Refs.[3,4,91-94,117]).

Analysis of the data in table 2.11 allows to make the following conclusions. Firstly, the accurate account of the complicated inter-electron (vacancy) correlations plays a critical role not only for acceptable quantitative agreement between theory and experiment, however, it is of the principal importance for right interpretation of the corresponding transitions in the spectra.

Table 2.11

The "i-f" transitions energies (in 10^2 cm^{-1}) , calculated within ab initio QED PT, MCDF and available experimental data.

N	i	f	Exp.[15]	MCDF	RPT	QED PT
1	$1s2s^22p^63s^23p$	$1s\ ^22s^22p^63s^2$	577000	577500	577200	577148
2	$1s2s^22p^63s^23p^2$	$1s\ ^22s^22p^63s^23p$	575700	576230	575910	575820
3	$1s2s^22p^63s^23p^3$	$1s\ ^22s^22p^63s^23p^2$	574400	575040	574940	574532
4	$1s2s^22p^63s^23p^4$	$1s\ ^22s^22p^63s^23p^3$	573400	573920	574360	573937
5	$1s2s^22p^63s^23p^5$	$1s\ ^22s^22p^63s^23p^4$	572400	572860	573520	572845
6	$1s2s^22p^63s^23p^6$	$1s\ ^22s^22p^63s^23p^5$	571430	571886	572550	572124

Secondly, usually acceptable [14] interpretation of the experimental highly ionized iron spectra, probably, is not fully correct because of the high complexness these spectra and, besides, using the DF calculation results for the corresponding interpretation. In fact in our opinion, the experimental data, in particular, for the "5" and "6" transitions (see table 2.11) are probably not correct and corresponding to other transitions. The difference between the RPT and QED PT data is connected with using the a little different basises of the relativistic wave functions. In ab initio approach calculation it has been used the QED procedure [128]. In refs. [93,94] it has been used the empirical zeroth approximation, which naturally accounts for the main (not all) part of the inter-particle correlations contribution. In table 2.12 we listed the values for probabilities of decay of the FeX states with vacancy $1s_{½}$, obtained within our approach (QED PT) with using the optimized basises (OB) of the one-quasiparticle wave functions and calculation data within the RPT with empirical zeroth approximation (without optimization of basises (WOB) of the wave functions) [128].

The analysis of the presented data in the table 2.2 shows that the QED PT results are less than the corresponding data from [94] at ~5%. This fact can be explained by using specially optimized basises of the one-quasiparticle wave

functions (more full account of multi-body exchange-correlation effects) in the EA scheme.

Table 2.12

Probabilities of decay of the FeX states with vacancy $1s_{1/2}$: QED PT –OB (A-QED PT data); RPT-WOB (B).

n_2l_2						
method	A	B	A	B	A B	A
n_1l_1	2s		2p		3s	3p
2s	399+14	42+14	131+14	14+15	130+14 14+14	198+14
2p			264+15	28+15	158+14 17+14	722+14
3s					834+12 90+12	243+13
3p						612+13

Note: the mantissa and decimal order of value are given: $42+14=0.42\cdot10^{14}$;
In refs. [91] it had been used the formalism of relativistic PT with the empirical zeroth approximation, and optimization of the one-quasi-particle wave functions basises is not specially fulfilled, though using the empirical information about corresponding one-quasiparticle atomic ion allows indirectly take into account the correlation corrections.

2.4 Autoionization resonances widths in YbI and TmI atoms

In table 2.14 we present the experimental data (Letokhov et al [101]) and theoretical results for energies and widths of the autoionization states of the 7*s*6*p* configuration on YbI(account from the ground state: $6s^2$ Yb): *E1*,*Γ1*- data by Ivanov et al (EA-RPTMP method); *E2*,*Γ2*- EA-QED PT data [101-107,126-129].

Table 2.13

Energies E (cm^{-1}) and widths *Γ* (cm^{-1}) of the YbI 7*s*6*p* configuration states

Term	Theory				Experiment	
	E1	*Γ1*	*E2*	*Γ2*	E_{exp}	Γ_{exp}
$^3P_0^0$	59800	0,70	59450	1,25	59130,5	1,1
$^3P_1^0$	60000	3,00	60315	1,10	60428,7	0,95
$^3P_2^0$	62600	0,70	62587	1,51	62529,1	1,6
$^1P_1^0$	63600	1,80	63613	2,48	63655,8	2,6

An analysis shows quite physically reasonable agreement between the values of energies E1, E2, E_{exp}, however, the values of the widths *Γ1*, Γ_{exp} significantly differ. 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.

The EA-QEDPT values [117,128] for widths are significantly closer to experimental data. It is connected with using more optimized basises of the orbitals and more accurate accounting for the important multi-body exchange-correlation effects. In table 2.14, 2.15 the autoionization states energies and widths for YbI with doubly excited valent shell are listed [101-107,126-129]: *E1,Γ1*- data by Ivanov et al (EA-RPTMP method); *E2,Γ2*- EA-QED PT data.

The presented EA-RPTMP and EA-QEDPT data for the energies are in the physically reasonable agreement with experimental data.

Table 2.14

Energies (in 10^2 cm-1) of autoionization states for Yb with 2-excited valent shell

Conf.	J	Theory		E_{exp}
		E1	*E2*	
$6p_{1/2}^2$	0	-1067	-1064	-1062,7
$6p_{3/2}^2$	0	- 920	- 918	—

	2	- 987	-1004	-1008,9
$6p_{1/2}6p_{3/2}$	1	-1054	-1050	-1049
	2	-1032	-1036	-1039,5
$6p_{1/2}5d_{3/2}$	1	-1077	-1072	—
	2	-1075	-1069	—
$6p_{1/2}5d_{5/2}$	2	-1007	-1004	—
	3	-1119	-1115	—
$6p_{3/2}5d_{3/2}$	0	-1020	-1017	—
	1	-1014	-1012	—
	2	- 914	- 913	—
	3	-1039	-1035	—
$6p_{3/2}5d_{5/2}$	1	- 949	- 948	—
	2	-1118	-1116	—
$6p_{3/2}5d_{5/2}$	3	- 963	- 962	—
	4	-1062	-1061	—
$5d_{3/2}^2$	0	- 981	- 982	—
	2	-1034	-1032	-101076
$5d_{5/2}^2$	0	- 961	- 963	—
	2	- 970	- 968	—
	4	- 861	- 859	—
$5d_{3/2}5d_{5/2}$	1	- 980	- 982	—
	2	- 994	- 995	-99463
	3	-1030	-1032	-103247
	4	-1024	-1026	—
$7s_{1/2}6p_{1/2}$	0	- 889	-886,4	—
	1	- 887	- 886	—
$7s_{1/2}6p_{3/2}$	1	- 851	- 849	—
	2	- 861	-860	—

Table 2.15

The widths (cm^{-1}) of autoionization states for Yb with doubly excited valent shell

Configurations	J	Term	$\Gamma 1$	$\Gamma 2$	Configurations	J	Term	$\Gamma 1$	$\Gamma 2$
$6p^2_{3/2}$	0	$^1S_0$	5.4	5.69	$6p_{3/2}5d_{3/2}$	2	$^1D_2^0$	0.20	0.52
	1	$^1P_1^0$	5.7	5.95	$5d_{3/2}5d_{5/2}$	1	$^3P_1$	1(-4)	8(-4)
$6p_{3/2}5d_{5/2}$	3	$^1F_3^0$	1.60	1.98	$5d^2_{5/2}$	0	$^1S_0$	3.30	3.63
$5d^2_{3/2}$	0	$^3P_0$	0.01	0.05	$5d^2_{5/2}$	2	$^3P_2$	0.40	0.73
						4	$^1G_4$	0.90	1.74

Note: 0.0008=8(-4)

However, comparison of the corresponding results for widths demonstrates again sufficiently large discrepancy. Analysis shows too that the state $5d_{3/2}5d_{5/2}$, (J=1) is really autoionizative (hitherto this question remained opened). Its anormal smallness can be explained by the fact that its decay is forbidden in the nonrelativistic limit. Further we consider the thulium atom, which is of a great interest for many physical and chemical applications [104-106]. In fig.2.1 we present position of nearly lying ionization limits $4f^{13}6snl$ of the thulium atom Tm and scheme of autoionization decay of the Tm Rydberg states $4f^{13}6snl$ [106,127]. Note that the availability of two pairs of near-lying ionization limits (with vacancy states $4f7^1/2$ and $4f5^1/2$) in the thulium atom provides two main types of the autoionization resonance decay [104-106,127].

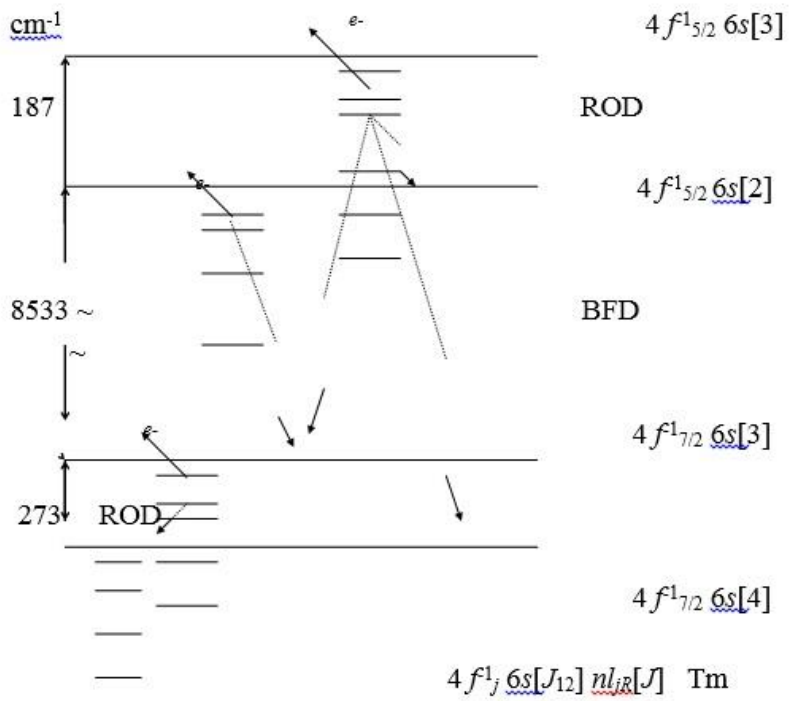

Figure 2.1 The position of nealy lying ionization limits $4f^{-13}6snl$ of the thulium atom Tm and scheme of autoionization decay of the Tm Rydberg states $4f^{13}6snl$ These decays are as follows:

(BFD) $4f^{-1}_{5/2}\ 6s1/2\ (J12)\ nl$ - $4f^{-1}_{7/2}\ 6s1/2\ [J12']\ Tm^{+} + leje,\ n>7,\ J12=2;\ 3,$ $J12'=3;\ 4$

(ROD) $4f^{-1}j6s1/2(J12)nl$-$4f^{-1}j6s1/2[J12']Tm^{+}$+$leje,\ n>25,\ J12=3,\ J12'=2;4$ $j=5/2,7/2$

Here the ROD means the reorientation autoionization resonance decay (new type of the autoionization decay developed Ivanov-Letokhov et al [101,106,127]), and the BFD means the traditional Beutler-Fano autoionization decay. The states $4f^{-1}_{5/2}\ 6s_{1/2}(J12=3)nl$ undergo simultaneously both BFD and ROD. Let us note that contrary to the BFD, the ROD is a low energy process preserving all the single electron quantum numbers of atomic residue: $4f^{-1}j$ and $6s_{1/2}$. The ROD can be of the monopole or quadruple character. We mean here the multi-polarity of the inter-quasi-particle interaction causing the autoionization resonance decay. The states with $J12=2;4$ do not undergo the ROD. Nevertheless, their admixing with states undergoing the ROD can significantly amplify the monopole ROD. For Rydberg series, the only possible autoionization resonance decay is the reorientation one. In table 2.16-2.19 we listed our calculated

values of the energies (E2) and widths (Γ2) for the autoionization states Tm $4f^{13}_{7/2}6s_{1/2}(3)ns_{1/2}[J]$, $4f^{13}_{7/2}6s_{1/2}(3)np_j[J]$ and $4f^{13}_{5/2}6s_{1/2}(2)ns_{1/2}[J]$, $4f^{13}_{5/2}6s_{1/2}(3)ns_{1/2}[J]$ Tm [120,127]. For comparison we also present the results of calculation by Ivanov etal (energy – E1; width -Γ1) [104-106]. Let us note that for the first states (see tables 2.16-2.18) the autoionization decay can be only realized by means of the ROD channel.

Table 2.16

The energies (in 10 cm^{-1}) and widths (cm^{-1}) of the autoionization states Tm $4f^{13}_{7/2}6s_{1/2}(3)ns_{1/2}[J]$

	J=5/2		*J=5/2*		*J=7/2*	*J=7/2*
N	Γ1	Γ2	E1	E2	Γ2	E2
25	1.18(-5)	1.29(-5)	4985	4964,3	1.63(-2)	4967.3
30	5.77(-6)	6.72(-6)	4995	4974.3	4.21(-3)	4976.5

Table 2.17

The energies (in 10 cm^{-1}) and widths (cm^{-1}) of the autoionization states Tm $4f^{13}_{7/2}6s_{1/2}(3)np_j[J]$

(j,J)	*(3/2,3/2)*		*(1/2,5/2)*		*(3/2,5/2)*	
N	Γ2	E2	Γ2	E2	Γ2	E2
25	5.24(-5)	4966,1	1.196(-1)	4965	1.95(-1)	4966,5
30	3.76(-5)	4975,5	9.23(-2)	4975,1	1.08(-1)	4975,7
(j,J)	*(1/2,7/2)*		*(3/2,7/2)*		*(3/2,9/2)*	
N	Γ2	E2	Γ2	E2	Γ2	E2
25	3.82(-2)	4964.0	3.56(-1)	4966,6	4.05(-1)	4966,9
30	2.54(-2)	4974.1	2.34(-1)	4975,8	2.67(-1)	4975,9

For the states in table 2.19 the autoionization decay can occur through both ROD and BFD channels, however it becomes to be possible only for states with n>25. A comparison of the presented theoretical data leads to conclusions, which were made for the ytterbium atom autoionization states. In conclusion of this point let us underline that the precized data on characteristics of the

Table 2.18

The energies (in 10 cm^{-1}) and widths (cm^{-1}) of the autoionization states Tm

$$4f_{5/2}^{13}6s_{1/2}(2)ns_{1/2}[J]$$

	J=3/2		*J=3/2*		*J=5/2*	*J=5/2*
n	Γ1	Γ2	E1	E2	Γ2	E2
10	4.23(-3)	4.61(-3)	5482	5464	5.33(-3)	5453
15	2.26(-4)	2.47(-4)	5763	5745	4.62(-4)	5748
25	2.48(-5)	2.75(-5)	5838	5821	5.61(-5)	5823
30	1.22(-5)	1.43(-5)	5847	5829	2.66(-5)	5830

Table 2.19

The energies (in 10 cm^{-1}) and widths (cm^{-1}) of the autoionization states Tm

$$4f_{5/2}^{13}6s_{1/2}(3)ns_{1/2}[J]$$

	Γ2 *J=5/2*			Γ2 *J=7/2*		
n	Γ(ROD)	Γ (BFD)	Γ (Total)	Γ(ROD)	Γ (BFD)	Γ (Total)
10		4.81(-3)	4.81(-3)		5.61(-3)	5.61(-3)
15		2.73(-4)	2.73(-4)		4.86(-4)	4.86(-4)
25	1.41(-2)	2.96(-5)	1.42(-2)	1.51(-5)	5.54(-5)	7.05(-5)
30	3.41(-3)	1.56(-5)	3.42(-3)	6.10(-6)	2.92(-5)	3.53(-5)

auotionization states for heavy atoms and ions (in our case, lanthanides atoms) are important not only from the point of view of the development of the advanced relativistic theory, however, from the point of view of the different apllications in laser physics, astrophysics, physics of plasma and development of new laser ionization technologies for the separation of the heavy isotopes, nuclear isomers etc.

2.5 The Tm, U autoionization resonance decay in a weak electric field and laser photoionization method of isotope separation

Now it is well known that the laser photoionization method is one of the most perspective methods for the sensing single atomic particles, separating isotopes, nuclear isomers and nuclear reactions products (see Refs. [162-191]). The

standard laser ionization (ALVIS) scheme may be realized by means of the multi-step excitation and ionization of atoms by laser pulse. The scheme of selective ionization of atoms, based on the selective resonance excitation of atoms by laser radiation into states near ionization boundary and further photo-ionization of the excited states by additional laser radiation, has been at first proposed and realized by Letokhov et al (see Refs. [162,172]). Naturally, this scheme if of a great interest in problem of the laser separation of isotopes and nuclear isomers. However, a significant disadvantage of the two-step selective ionization of atoms by laser radiation method is a great difference between cross-sections of resonant excitement σ_{exc} and photo-ionization σ_{ion} ($[\sigma_{exc}/\sigma_{ion}]>10^4\div10^8$). It requires using very intensive laser radiation for the excited atom ionization. The situation is more simplified for autoionization resonances in the atomic spectra, but detailed data about characteristics of these levels are often absent. Main problems here are connected with difficulties of theoretical studying and calculating the autoionization resonance characteristics (see above). An account of complex relativistic and correlation effects (continuum states, exchange-correlation effects etc) by means of the traditional quantum-mechanical methods is not possible hitherto [1-4].

In a number of papers (see Refs. [172,175,191]) a possibility of the selective ionization of atoms, based on the selective resonance excitation of atoms by laser radiation into states near ionization boundary and further ionization decay of excited atoms by external electric field, has been considered. Electric field changes the electron spectra so that the part of discrete spectra levels (near the ionization boundary) moves into continuum and other levels become the autoionization ones.

The probability of their autoionization decay quickly increases with growth of the main quantum number. The most optimal situation is when atom is excited to state, which has the autoionization probability more than the radiation decay probability.

To receive a précised information about optimal laser photoionization scheme, it is necessary to carry out an accurate calculation of the process of sequent atomic excitation by laser field (it's known trivial task) and probability of ionization of the atoms in the highly excited states (autoionization states) by electric field.

As a rule, non-relativistic approximation has been earlier used [175]. More consistent approach to solution of such a problem must be based on the relativistic models [117-160], as the most interesting elements for laser isotope separation are heavy isotopes, where a role of relativistic corrections is often very dramatic. Below we use a relativistic energy approach for numeral calculation of the autoionization resonances decay in the external DC electric field [126-128].

It should be also noted that studying the autoionization in an external DC electric field represents an undoubted interest for experimental laser spectroscopy, in controlling the population and decay kinetics of excited states or the selective ionization under laser radiation action [191]. One could mention a great role of the autoionization resonances in many processes in plasma and gases. The corresponding data can be very useful for carrying out optimal isotope separation scheme. Really, according to Ref. [191], an effective optimized isotope separation scheme can be based on the selective laser excitation of the isotope atom into the excited Rydberg states and further DC electric field ionization or autoionization. In this case the velocity of ionization is significantly higher than the corresponding value in the usual regime (see Refs. [172,175]). A result, the effectiveness of the laser photoionization scheme of isotope separation is significantly increased. As example let us consider a process of the uranium *U* and thulium *Tm* isotopes separation [72,120,151,152].

The necessary ionization step: excitation of the uranium and thulium atoms into the Rydberg states: $5f^3 7s^2 np$, $5f^3 6d7sns$ (*U*: electron external shell configuration) and $4f^{13} 6sns$, $4f^{13} 6snp$ (*Tm*). Principal quantum number n may be equal 10-50. The further step is an autoionization decay in an external DC electric field. It should be noted that the excitation and ionization cross-sections of ground and low excited state for these atoms by laser pulse are as follows: the excitation cross-section $\sigma_{exc}=\sigma_1$ ~10^{-13}-10^{-11} cm^2, ionization cross-section from excited state: $\sigma_{ion}=\sigma_2$~10^{-18}-10^{-17}cm^2, from ground state σ_2~10^{-19}cm^2 [175,191]. For selective photoionization scheme with excitation to Rydberg *ns, np* states with *n*=10-50 and further ionization by the DC electric field (see below) the calculated cross-section values are as follows: σ_2~$\cdot 10^{-15\div 12}$ cm^2. It means that the selective photoionization scheme with using the Rydberg states (autoionization resonances) and ionization by external electric field is more effective for studied

isotopes from the energetic point of view. But it is arisen a problem with the ionization output (here it may be less than 100%, so it is necessary to search the optimal levels). To get the corresponding data on probabilities of ionization by external DC electric field, one could use a consistent relativistic quantum approach to calculation of the autoionization resonance decay in the external DC electric field [126-127,151,152].

Probability of the ionization (autoionization width) for highly excited atoms by electric field is given by the full flow of probability through the plane, which is perpendicular to z-axe. Calculation of the probability requires a solution of the axially symmetrical problem, when a potential barrier separates two classically allowed regions. To define the wave functions and electron state energies in an electric field, one needs to carry out the diagonalization of energy matrice, calculated between states with the same n [126-129].

The diagonalization of the complex energy matrix leads to complex energy correction: ReE -iΓ/2 , where Re E is the level shift and Γ is the level width, including the radiation and autoionization widths simultaneously. If the effects of the autoionization resonance decay are included in the matrix M, then Γ presents only the autoionization width of the state.

Only Re M is diagonalized. The imaginary part is converted by means of the matrix of eigen-vectors $\{C_{mk}\}$ The eigen vectors are obtained by diagonalization of ReM (see formular (62)). The other details of calculation procedure can be found in Refs. [117-160]. From physical point of view, especially interesting effects occur in the complex heavy atom when its broad autoionization resonances mix with much narrower resonances of opposite parity by means the external electric field. Here the most interesting feature is an effect of electric field on the autoionization resonances in the heavy isotopes (the last step of the laser photoionization scheme).

Authors of paper [126,128] have predicted new effect, connected with behaviour of the Tm autoionization resonances in an external electric field and discovered a drastic broadening of the reorientation type autoionization resonances already in a weak electric field. We have carried out the same calculation, but with the use of the relativistic energy approach. It is easy understand that any two states of different parity can be mixed by the external electric field. The mixing leads to redistribution of the autoionization widths. In the case of degen-

erate or near-degenerate resonances this effect becomes observable even at a moderately weak field. In the case of the thulium one could deal with reorientationally decaying *ns* and *np* series, converging to the same ionization limit, i.e. they are nearly degenerate states of different parity. Among them one can find some pairs of *ns* and *np* states with widths Γ, differing by several orders (see fig. 2.1).

As example, we consider the $f^{-1}{}_{7/2}$ 6*s*(3)25*s*[5/2] state, decaying due to the quadruple interaction and $f^{-1}{}_{7/2}$ 6*s*(3)25$p_{1/2}$[5/2] undergoing to the monopole ROD. In table 2.20 we present the calculated values of the energy *E*, autoionization width Γ for the $4f7^{-1}/26s(3)ns,np$ Tm states (*n*=25) for different values of the DC electric field strength ε. A strong change of the autoionization resonance width occurs at a moderately weak electric field and presented data are fully corresponding to the pioneering data by Glushkov-Ivanov [126].

Table 2.20

The calculated values of the autoionization width Γ (cm^{-1}) for the $4f7^{-1}/26s(3)ns,np$ Tm states (*n*=25) for different values of DC electric field strength ε. ($V \cdot cm^{-1}$)

State	$4f^{13}{}_{7/2}$ 6*s*1/2 (3) 25*s* [5/2]	$4f^{13}{}_{7/2}$ 6*s*1/2 (3) 25$p_{1/2}$ [5/2]
Γ, ε = 0	1,291D – 05	1,196D – 01
Γ, ε = 50	1,847D – 04	1,194D – 01
Γ, ε = 100	7,130D – 04	1,189D – 01
Γ, ε = 150	1,330D –03	1,182D - 01

The same effect is firstly discovered by us for the uranium isotopes. We have calculated the energies and widths for higher members of the uranium Rydberg series (members accessed from 32.899,79 cm^{-1} level). Excitation sequence: 6056,81+6098,10+(5880-5890) Å. For $5f^37s^2np$ *(n=40-44)* levels the following results are obtained: i). For ε=0 $V \cdot cm^{-1}$, configuration $5f^37s^242p$, *E*=49877,49 (experimental value [13]: 49877,5); $\Gamma(5f^37s^242p)$=1,794D-01; $\Gamma(5f^37s^242s)$= 2,702D-05; ii). For ε = 100 $V \cdot cm^{-1}$; $\Gamma(5f^37s^242p)$=1,675D-01; $\Gamma(5f^37s^242s)$=

5,913D-04. So, we have here a strong change of the autoionization resonance width at a moderately weak electric field too. In conclusion let us underline here that the detailed spectroscopic information about autoionization resonances is needed to optimize the excitation and ionization of the atom. An optimal scheme presumes a compromise between high excitation probability and high decay rate that determines the lower and upper boundaries for the autoionization resonances decay rate. The use of the autoionization decay (for example, the ROD channel) essentially increases the possibilities of such a compromise. As example, here we briefly consider possible optimal laser photoionization scheme of the uranium isotope separation. As usually [151,152], the optimization procedure of the laser photoionization scheme is in a searching the optimal form of the laser pulse to provide a maximum of excited particles in the separation scheme (naturally this is one of the possible versions).

The whole separation process is described by the density matrice equations system [191]. The laser photoionization scheme for *U* isotopes includes the following steps: i). Laser excitation of the ^{235}U isotopes from the ground $5f^36d7s^2\text{-}^5L_6^o$ state and low lying metastable $5f^36d7s^2\text{-}^5K_5^o$ state with energy 620,32 $см^{-1}$; ii). Transition into the autoionization state with doubly excited external shell and then ionization by the DC electric field.

In figure 2.2 we present the results of numerical modelling the optimal form of laser pulse in the laser photoionization sensor scheme for the uranium isotopes (from Ref. [151]). The following notations are used: δ pulse + dotted line is the optimal form of the laser pulse; curves (1) x_1 ,(2) x_2 are populations of the ground and excited (n=42) states.

At the first step of the laser photoionization scheme the δ-pulse provides a maximally possible level of excitation for the upper states. At the last step an external DC electric field ionization must be realized earlier than the parasitic spontaneous relaxation processes (resonant re-charging etc. [175,191]) begin to destroy and change the reached level of atomic excitation. Using the DC electric filed ionization mechanism significantly increases the output of charged particles, improves in whole the energetics of the laser photoionization sensor scheme and its optimality. It is possible to accept the special measures to provide very high ionization output (approaching to 100%) that requires using specially separated autoionization levels.

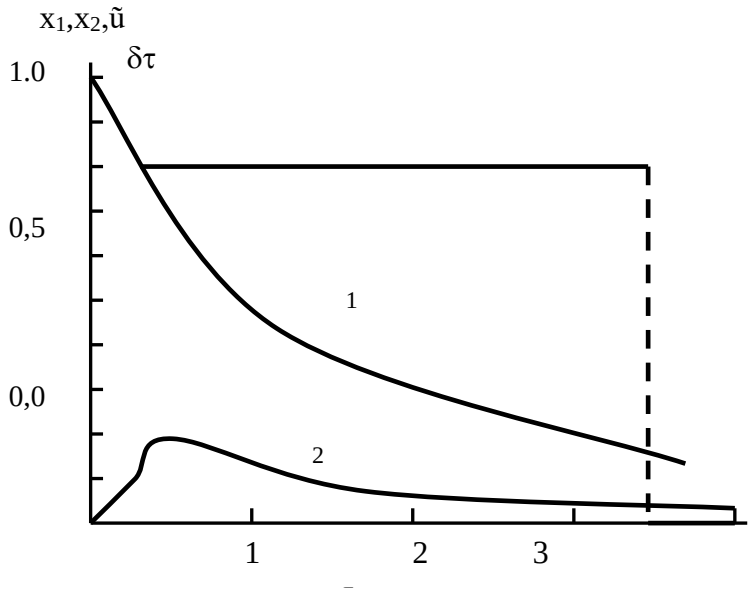

Figure 2.2 Results of numerical modelling for the optimal form of laser pulse in the laser photoionization sensor scheme for the uranium isotopes: δ pulse + dotted line is the optimal form of the laser pulse; curves (1) x_1 and (2) x_2 are the populations of the ground and excited states.

General analysis shows [191] that described laser photoionization scheme is more perspective for uranium in comparison to traditional two- and three-step laser photoionization schemes with ionization by laser pulse at the final step [175,180-190].

2.6 Conclusions

We presented the generalized QED energy approach to relativistic calculation of the radiative and autoionization characteristics for multielectron atoms and ions. The approach is based on the Gell-Mann and Low S-matrix formalism and the gauge-invariant QED perturbation theory (PT) with using the optimized one-quasiparticle representation and an accurate account of the relativistic, correlation, nuclear and even radiative effects. In relativistic case the Gell-Mann and Low formula expressed an energy shift through the QED scattering matrix including the interaction with as the laser field as the photon vacuum field. The last case is corresponding to definition of the traditional radiative characteristics of atoms and ions. The results of relativistic calculation of the radiative transi-

tions probabilities, oscillators strengths, autoionization widths are (some part firstly) presented for a number of heavy atoms and multicharged ions and discussed from the point of view of the correct accounting for the relativistic and exchange-correlation effects. Besides, some important possible applications, in particular, searching optimal schemes for laser photoionization isotope separation method with using the autoionization and DC electric field ionization mechanisms are briefly considered.

References

1. Glushkov A.V., Advanced Relativistic Energy Approach to Radiative Decay Processes in Multielectron Atoms and Multicharged Ions// Quantum Systems in Chemistry and Physics: Progress in Methods and Applications. Series: Progresss in Theoretical Chemistry and Physics, Eds. K.Nishikawa, J. Maruani, E.Brandas, G. Delgado-Barrio, P.Piecuch (Berlin, Springer).-2013-Vol.26.-P.231-254;
2. Khetselius O.Yu., Relativistic energy approach to cooperative electron-gamma-nuclear processes: NEET Effect// Quantum Systems in Chemistry and Physics: Progress in Methods and Applications. Series: Progresss in Theoretical Chemistry and Physics, Eds. K.Nishikawa, J. Maruani, E.Brandas, G. Delgado-Barrio, P.Piecuch (Berlin, Springer).-2012-Vol.26.-P.217-230.
3. K.G. Dyall, K. Faegri, Jr. *Introduction to Relativistic Quantum Theory* (Oxford University Press, Oxford, 2007); I.P. Grant, *Relativistic Quantum Theory of Atoms and Molecules, Theory and Computation, Springer Series on Atomic, Optical, and Plasma Physics*, vol. 40 (Springer, Berlin, 2007), p. 587–626
4. A.V. Glushkov, *Relativistic and Correlation Effects in Spectra of Atomic Systems* (Nauka, Moscow-Odessa, 2006), 550p.
5. A.V. Glushkov, *Relativistic Quantum Theory. Quantum Mechanics of Atomic Systems* (Astroprint, Odessa, 2008), 900p.
6. I.P. Grant, H.M. Quiney, Int. J. Quant. Chem**. 80**, 283–297 (2000) ; K.L. Bell, K.A. Berrington, D.S.F. Crothers, A. Hibbert, K.T. Taylor, *Bertha: 4-Component Relativistic Molecular Quantum Mechanics, in Supercomputing, Collision Processes, and Application*, Series: *Physics of Atoms and Molecules*, (Kluwer, New York, 1999) pp. 213–224.
7. M. Reiher, B. Hess, in *Modern Methods and Algorithms of Quantum Chemistry,* ed. by J. Grotendorst, John von Neumann Institute for Computing, Julich, NIC Series, vol 3, (2000) pp. 479–505.
8. H.M. Quiney, in *Relativistic Quantum Mechanics of Atoms and Molecules. New Trends in Quantum Systems in Chemistry and Physics*, Series:

Progress in Theoretical Chemistry and Physics, vol 6 (Springer, Berlin, 2002) pp. 135–173.

9. S. Wilson, Journ. of Mol. Str.: Theochem. **547**, 279–291 (2001)
10. I.P. Grant, H.M. Quiney, Int. J. Quantum Chem. **80**, 283 (2000)
11. *Advanced Topics in Theoretical Chemical Physics,* Series: *Progress in Theoretical Chemistry and Physics*, vol. 12, ed. by J. Maruani, R. Lefebvre, E. Brändas (Springer, Berlin, 2004)
12. *H.Jensen, T.Saue, L.Visscher with contr. by V.Bakken, E.Eliav, T. Enevoldsen, T.Fleig, O.Fossgaard, T.Helgaker, J.Laerdahl, C.Larsen, P. Norman, J.Olsen, M.Pernpointner, J.Pedersen, K.Ruud, P.Salek, J. van Stralen, J.Thyssen,O. Visser, T.Winther, DIRAC Code, a relativistic ab initio electronic structure program, Release DIRAC4.0.-2004; (*http://dirac.chem.sdu.dk*).*
13. *W.*Martin, *NIST Spectra Database, version 2.0,* NIST, Washington,2004; *(http:// physics.nist.gov.asd).*
14. *C. Moore, NBS Spectra Database,* NBS, Washington, 1987.
15. A.V. Glushkov, S.V. Ambrosov, A.V. Loboda, E.P. Gurnitskaya, O.Yu. Khetselius, in *Recent Advances in Theoretical Physics and Chemistry Systems*, Series: *Progress in Theoretical Chemistry and Physics*, vol. 15, ed. by J.-P. Julien, J. Maruani, D. Mayou, S. Wilson, G. Delgado-Barrio (Springer, Berlin, 2006), pp. 285-300.
16. A.V. Glushkov, O.Yu. Khetselius, E.P. Gurnitskaya, A.V. Loboda, T.A. Florko, D.E. Sukharev, L. Lovett, in *Frontiers in Quantum Systems in Chemistry and Physics*, Series: *Progress in Theoretical Chemistry and Physics*, vol. 18, ed. by S. Wilson, P.J. Grout., J. Maruani, G. Delgado-Barrio, P. Piecuch (Springer, Berlin, 2008), p.501-522
17. A.V. Glushkov, O.Yu. Khetselius, L. Lovett, L., in: *Advances in the Theory of Atomic and Molecular Systems Dynamics, Spectroscopy, Clusters, and Nanostructures*. Series: *Progress in Theoretical Chemistry and Physics*, vol. 20, ed. by P.Piecuch, J. Maruani, G. Delgado-Barrio, S. Wilson (Springer, Berlin, 2010), pp.125-172.
18. A.V. Glushkov, S.V. Ambrosov, A.V. Loboda, Yu.G. Chernyakova, O.Yu. Khetselius, A.A. Svinarenko, Nucl. Phys. A **734**S, 21 (2004)
19. A.V.Glushkov, S.V.Malinovskaya, O.Yu. Khetselius, D.E.Sukharev,

A.V.Loboda, L.Lovett, Int. Journ. of Quant.Chem. **109**, 1417 (2009).

20. *Photonic, Electronic and Atomic Collisions*, ed. by F. Aumar and H. Winter (World Scientific, Singapore, 1997), pp.1-650.
21. M. Hehenberger, H. McIntosh, E. Brändas, Phys. Rev. A **10**, 1494 (1974).
22. E.Brändas, P. Floelich, Phys. Rev.A **16**, 2207 (1977).
23. J.C. Slater, *The Consistent Field Method for Molecules and Solids: Quantum Theory of Molecules and Solids*, vol. 4 (McGraw-Hill, New York, 1974).
24. S. Wilson, in *Recent Advances in Theoretical Physics and Chemistry Systems*, Series: *Progress in Theoretical Chemistry and Physics*, vol. 16, ed. by J. Maruani, S. Lahmar, S. Wilson, G. Delgado-Barrio (Springer, Berlin, 2007), p. 11-80.
25. S. Wilson, *Handbook on Molecular Physics and Quantum Chemistry* (Wiley, Chichester, 2003).
26. I. Theophilou, S. Thanos, A. Theophilou, J. Chem. Phys. **127**, 234103 (2007).
27. D.J. Dean, M. Hjorth-Jensen, K. Kowalski, P. Piecuch, M. Wloch, in *Condensed Matter Theories*, ed. by J.W. Clark, R.M. Panoff, H. Li (Nova Sci. Publishers, 2006).
28. P. Piecuch, M. Wloch, J.R. Gour, D.J. Dean, M. Hjorth-Jensen, T. Papenbrock, in *Nuclei and Mesoscopic Physics: Workshop on Nuclei and Mesoscopic Physics* WNMP 2004, AIP Conference Proceedings, vol. 995, ed. by V. Zelevinsky (American Institute of Physics, Melville, NY, 2005), p. 28.
29. W. Kohn, L.J. Sham, Phys. Rev. A **140**, 1133 (1964).
30. P. Hohenberg, W. Kohn, Phys. Rev. B **136**, 864 (1964).
31. E.G. Gross, W. Kohn, *Exchange-Correlation Functionals in Density Functional Theory* (Plenum, New York, 2005).
32. *The Fundamentals of Electron Density, Density Matrix and Density Functional Theory in Atoms, Molecules and the Solid State*, Series: *Progress in Theoretical Chemistry and Physics*, vol. 14, eds. N. Gidopoulos and S. Wilson (Springer, Berlin, 2004), p.1.
33. R.M. Dreizler, Phys. Scripta T **46**, 167 (1993).
34. E.Clementi, C.Roetti, Atom. Data Nucl. Data Tables. **14**, 177 (1974).

35. C.Froese Fischer, G.Tachiev, Atom. Data Nucl. Data Tables. 87, 1 (2004).
36. C.Froese Fischer, G.Tachiev, A. Irimia, GAtom. Data Nucl. Data Tables. 92, 607 (2006).
37. E.Luc-Koenig, A. Lyras, J.-M. Lecomte, M. Aymar, J.Phys. B: At. Mol. Opt. Phys. **30**, 5213 (1997).
38. M.A.Klapish, Comp.Phys.Commun. **2**, 239 (1971).
39. C.Laughlin, G.A. Victor, Adv. Atom. Mol. Phys. **25,** 163 (1988).
40. P.Durand, J.Malrieu, *Ab initio quantum chemistry methods* Wiley, New York, 1987).
41. J.Bieron, C.Froese-Fischer, S.Fritzsche, K. Pachucki, J.Phys.B:At.Mol.Opt.Phys. **37**, L305 (2004).
42. K.N. Koshelev, L.N. Labzowsky, I.I. Tupitsyn, J. Phys. B **37**, 843 (2004)
43. J. Bieron, P. Pyykkö, P. Jonsson, Phys. Rev. A **71**, 012502 (2005).
44. J. Bieron, P. Pyykkő, Phys. Rev. A **71**, 032502 (2005).
45. P. Mohr, Atom. Data Nucl. Data Tabl**. 24**, 453 (1993); Phys. Scripta T **46**, 44 (1993).
46. M.P. Das, M.V. Ramana, A.K. Rajagopal, Phys. Rev. **22**, 9 (1980).
47. K. Cheng, Y. Kim, J. Desclaux, Atom. Data Nucl. Data Tabl. **24**, 11 (1979).
48. G. Drake, Phys. Scripta T **46**, 116 (1993).
49. H.M. Quiney, I.P. Grant, Phys. Scripta T **46**, 132 (1993).
50. G. Gould, Phys. Scripta T**46**, 61 (1993).
51. S. Blundell, Phys. Scripta T **46,** 144 (1993).
52. C.Froese-Fischer, Phys.Rev.A**39**, 963 (1989).
53. A.Weiss, J.Quant.Spectr. Radiat.Transf. **18**, 481 (1977).
54. W.R.Johnson, C.D.Lin, K.T.Cheng, Phys.Scr. **21**, 409 (1980).
55. W.R.Johnson, J.Sapistein, S.Blundell, Phys.Rev.A**37**, 307 (1988).
56. W. Johnson, J. Sapirstein, S. Blundell, Phys. Scripta 46, 184 (1993).
57. P. Indelicato, J.P. Desclaux, Phys. Scripta T **46**, 110 (1993)
58. V. Dzuba, V. Flambaum, P. Silvestrov, O. Sushkov, Phys. Rev. A **44**, 2828 (1991).
59. H. Persson, I. Lindgren, S. Salomonson, Phys. Rev. Lett. **76**, 204 (1996).
60. S.N. Tiwary, Rivista del Nuovo Cimento **18**, 1 (1995).
61. J. Bieron, C. Froese-Fisher, S. Fritzsche, K. Pachucki, J. Phys. B: At.

Mol. Opt. Phys. **37**, L305 (2004).
62. U. Safranova, T. Cowan, M. Safranova, J. Phys. B: At. Mol. Phys. **38**, 2741 (2005).
63. V. Dzuba, V. Flambaum, M.S. Safranova, Phys. Rev. A **73**, 022112 (2006)
64. W.R. Johnson, U.I. Safranova, M.S. Safranova, Phys. Rev. A.**67,** 062106 (2003).
65. U.I. Safranova, M.S. Safranova, W.R. Johnson, Phys. Rev. A **71**, 052506 (2005).

66. M.S.Safronova, W.R. Johnson, U.I. Safranova, T.Cowan, Phys.Rev.A.**74**, 022504 (2006).
67. U.I. Safranova, M.S. Safranova, S.M.Hamasha, P.Beiersdorfer, Atom. Data Nucl. Data Tabl. **92**, 47 (2006).

68. V. Yerokhin, A.N. Artemyev, V.M. Shabaev, Phys. Rev. A **75**, 062501 (2007)
69. B. Sahoo, G. Gopakumar, R. Chaudhuri, B. Das, H. Merlitz, U. Mahapatra, D. Mukherjee, Phys. Rev. A **68**, 040501 (2003)
70. J. Santos, F. Parenre, S. Boucard, P. Indelicato, J. Desclaux, Phys. Rev. A **71**, 032501 (2005)
71. A. Derevianko, S.G. Porsev, Phys. Rev. A **71**, 032509 (2005)
72. O.Yu. Khetselius, Phys. Scripta. T.**135**, 014023 (2008).
73. O.Yu. Khetselius, Int. Journ.Quant.Chem. **109**, 3330 (2009).
74. M.J.Jamieson, G.W.F.Drake, A.Dalgarno, Phys.Rev. A **51,** 3358 (1995).
75. L.Curtis, Phys.Rev.A**35**, 2089 (1987).
76. B.Saha, S.Fritzsche, J.Phys. B: At. Mol. Opt. Phys.**38**, 1161 (2005).
77. A.Hibbert, J.E.Hansen// J.Phys. B: At. Mol. Opt. Phys. **27**, 3325 (1994).
78. M.D.Kunisz, Acta Phys.Polon.A **62**, 285 (1982).
79. M. Grance, Atomic Data. **5**, 185 (1973).
80. W.C.Jupen, B.Denne, I.Martinson, Phys.Scripta. **41,** 669 (1990).
81. J.Migdalek, Can.J.Phys. **54,** 130 (1976).
82. V.N. Ostrovsky, S.A.Sheynerman, Opt. Spectr. (USSR) **67**, 16 (1989).
83. S.A.Kotochigova, Opt.Spectr. (USSR) **55**, 422 (1983).

84. S.L.Mandelstam, E.V.Aglitsky, P.S.Antsiferov, A.M.Panin, Canad. J.Phys. 62, 1923 (1984).
85. E.K.Anderson, E.M.Anderson, Opt.Spectr. (USSR). **54,** 955 (1983).
86. P. Quinet, C. Argante, V. Fivet, C. Terranova1, A. V. Yushchenko, É. Biémont, Astrophys. Astron. **474**, 307 (2007).
87. É. Biémont, V. Fivet, P. Quinet, J.Phys. B: At. Mol. Opt. Phys 37, 4193 (2004).
88. Bieron, J., Froese Fischer, C., Fritzche, S., & Pachucki, K. J.Phys. B: At. Mol. Opt. Phys 37, L305 (2004).
89. L.N. Labzovsky, JETP, **57**, 663 (1969); M.A.Braun, Yu.Yu.Dmitriev, L.N.Labzovsky, JETP. **57,** 2189 (1969).
90. L.N.Ivanov, E.P.Ivanova, Atom.Data Nucl. Data Tabl. **24**, 95 (1979).
91. L.N.Ivanov, M.N.Driker, Opt.Spectr. (USSR) **49**, 209 (1980).
92. M.N.Driker, E.P.Ivanova, L.N. Ivanov, A.F.Shestakov, J.Quant.Spectr. Rad.Transf. **28, 531 (**1982).
93. E.P. Ivanova, L.N. Ivanov, A.V. Glushkov, A. Kramida, Phys. Scripta **32**, 512 (1985).

94. E.P. Ivanova, A.V. Glushkov, J. Quant. Spectr. Rad. Transfer. **36**, 127 (1986).
95. L.N. Ivanov, V.S. Letokhov, JETP **68**, 748 (1975); JETP **71**, 19 (1976).
96. L.N. Ivanov, V.S. Letokhov, Com.Mod.Phys.D.:At.Mol.Phys. **4**, 169 (1985).
97. A.V. Glushkov, E.P. Ivanova, in: *Spectroscopy of multicharged ions*, ed. U.I.Safronova (Nauka, Moscow, 1986), pp.5-195.
98. A.V. Glushkov, S.V.Malinovskaya, Opt. Spectr. (USSR) **62**, 966 (1987); **62**, 1212 (1987).
99. A.V. Glushkov, Opt. Spectr. (USSR) **64,** 446 (1988); **65,** 1175 (1988).
100. A.V. Glushkov, S.V.Malinovskaya, in: *Many-body effects in atoms*, ed. U.I.Safronova (Nauka, Moscow, 1988), pp.73-189.
101. E.Vidolova-Angelova, L.N.Ivanov, E.P.Ivanova, V.S.Letokhov, Izv. AN USSR. Ser. Phys. **45**, 2300 (1981).
102. G.I. Bekov, E.Vidolova-Angelova, L.N.Ivanov, E.P.Ivanova, V.S.Letokhov, V.I.Mishin, JETP. **80,** 866 (1981).

103. E.Vidolova-Angelova, L.N.Ivanov, E.P.Ivanova, Opt. Spectr. (USSR). **50,** 243 (1981); Opt. Spectr. (USSR). **54**, 590 (1983).
104. E.Vidolova-Angelova, L.N.Ivanov, E.P.Ivanova, D.A.Angelov, J.Phys.B: At. Mol. Opt. Phys.**19,**-2053 (1986).
105. E.Vidolova-Angelova, L.N.Ivanov, J. Phys.B:At.Mol.Opt.Phys. **21**, 3877 (1988).
106. E.Vidolova-Angelova, L.N.Ivanov, J. Phys.B:At.Mol.Opt.Phys. **24**, 4147 (1991).
107. A.V. Glushkov, Sov. Phys. J. **40,** 34 (1991); **41** (N9)**,** 3 (1992).
108. L.N. Ivanov, E.P. Ivanova, JETP. **110**, 483 (1996)
109. E.P. Ivanova, L.N. Ivanov, E.V. Aglitsky, Phys. Rep. **166**, 315 (1988).
110. L.N. Ivanov, E.P. Ivanova, L. Knight, Phys. Rev. A **48,** 4365 (1993)
111. K.N. Koshelev, L.N. Ivanov, Phys. Rev. A **42**, 5784 (1990)
112. E.P. Ivanova, A.V.Gulov, Atom.Data.Nucl.Data.Tabl. **49**, 1 (1991).
113. E.P.Ivanova,A.Gogava, in: *Spectroscopy of autoionization states for atoms and ions*, ed. U.I.Safronova (Nauka, Moscow, 1988), pp.212-256.
114. E.P. Ivanova, I.P. Grant, J. Phys.B:At.Mol.Opt.Phys. **31**, 2871 (1998).
115. E.P. Ivanova, N.A. Zinoviev, Quant. Electronics **29**, 484 (1999).
116. E.P.Ivanova, N.A.Zinoviev, Phys. Lett.A. ,Vol.**274**, 239 (2001).
117. A.V. Glushkov, L.N. Ivanov, E.P Ivanova, *Autoionization Phenomena in Atoms*, (Moscow University Press, Moscow, 1986) pp.152-164.
118. A.V. Glushkov, J. Appl. Spectr. **52,** 297 (1990); **56,** 13 (1992); **56,** 482 (1992).
119. A.V. Glushkov, Opt. Spectr. (USSR). **66**, 31 (1989); **66**, 1180 (1989); **70**, 952 (1991).
120. A.V. Glushkov, Opt. Spectr. (USSR) **71**, 395 (1991); **72,** 55 (1992); **72,** 542 (1992).
121. A.V. Glushkov, JETP Lett. 55, 97 (1992).
122. A.V. Glushkov, Rus. J. Struct. Chem. **31**, 9 (1990); **32**, 11 (1992); **34**, 3 (1993).
123. A.V. Glushkov, Rus. J. Phys. Chem. **66**, 589 (1992); **66**, 1259 (1992).
124. A.V. Glushkov, L.N. Ivanov, Preprint of Institute for Spectroscopy of USSR Academy of Sciences (ISAN), AS N1 (ISAN, Moscow-Troitsk, 1992), pp.1-16.

125. A.V. Glushkov, L.N. Ivanov, Preprint of Institute for Spectroscopy of USSR Academy of Sciences (ISAN), AS N2 (ISAN, Moscow-Troitsk, 1992), pp.1-10.
126. A.V. Glushkov, L.N. Ivanov, Preprint of Institute for Spectroscopy of USSR Academy of Sciences (ISAN), AS N3 (ISAN, Moscow-Troitsk, 1992), pp.1-12.
127. A.V. Glushkov, L.N. Ivanov, V.S.Letokhov, Preprint of Institute for Spectroscopy of e USSR Academy of Sciences (ISAN), AS N4 (ISAN, Moscow-Troitsk, 1992), pp.1-16.
128. A.V. Glushkov, L.N. Ivanov, Phys. Lett. A **170**, 33 (1992);
129. A.V.Glushkov, S.V.Malinovskaya, Sov. Phys. J. **41 (**N11), 3 (1992).
130. A.V. Glushkov, L.N. Ivanov, Atomic Spectroscopy (Inst. Chem.Phys. AS, Chernogolovka, 1992), p.113.
131. A.V. Glushkov, L.N. Ivanov, J. Phys. B: At. Mol. Opt. Phys. **26,** L379 (1993)
132. A.V.Glushkov, S.V.Malinovskaya, S.V.Ambrosov, in: *Atomic Spectra and Oscillator Strengths for Astrophysical and Laboratory Plasmas* (Publ.de l'Observatoire de Paris, Meudon, 1996), pp.96-101.
133. A.V. Glushkov, in *Low Energy Antiproton Physics:* Eighth International Conference on Low Energy Antiproton Physics (LEAP '05), AIP Conference Proceedings, vol. 796, ed. by D. Grzonka, R. Czyzykiewicz, W. Oelert, T. Rozek, P. Winter (American Institute of Physics, Melville, NY, 2005), p. 206-215.

134. A.V. Glushkov, O.Yu. Khetselius, A.V. Loboda, E.P. Gurnitskaya, in *Meson-Nucleon Physics and the Structure of the Nucleon*, ed. by S. Krewald, H. Machner (IKP, Juelich, Germany), SLAC eConf C070910 (Menlo Park, CA, USA) **2**, 186 (2007); A.V.Glushkov, ibid. **2**, 111 (2007)
135. A.V. Glushkov, S.V. Malinovskaya, L.A.Vitavetskaya, Yu.V. Dubrovskaya, O.Yu. Khetselius, in: *Recent Advances in Theoretical Physics and Chemistry Systems*, Series: *Progress in Theoretical Chemistry and Physics*, vol. 15, ed. by J.-P. Julien, J. Maruani, D. Mayou, S. Wilson, G. Delgado-Barrio (Springer, Berlin, 2006), pp. 301-318.
136. A.V. Glushkov, S.V. Malinovskaya, Rus. J. Phys. Chem. **62**, 100 (1988).

137. A.V. Glushkov, S.V. Malinovskaya, Rus. J. Phys. Chem.**62**, 2970 (1988).
138. A.V. Glushkov, S.V. Malinovskaya, in *New Projects and New Lines of Research in Nuclear Physics*, ed. by G. Fazio, F. Hanappe (World Scientific, Singapore, 2003), pp.242-264.
139. A.V.Glushkov, O.Yu. Khetselius, in: *Nuclear Physics in Astrophysics* NPA-III (Dresden, Germany, 2007), p. 95; J. Phys. G., to be published.
140. A.V. Glushkov, S. Malinovskaya, A. Loboda, G. Prepelitsa, J. Phys.: Conf. Ser. **35**, 420 (2006)
141. A.V. Glushkov, S. Malinovskaya, E. Gurnitskaya, O. Khetselius, J. Phys.: Conf. Ser. **35**, 426 (2006)
142. A.V. Glushkov, S.V. Malinovskaya, A.V. Loboda, E.P. Gurnitskaya, D.A. Korchevsky, J. Phys.: Conf. Ser. **11**, 188 (2005)
143. A. Glushkov, S. Malinovskaya, G. Prepelitsa, V. Ignatenko, J. Phys.: Conf. Ser. **11**, 199 (2004)
144. A.V. Glushkov, I.T. Makarov, E. Nikiforova, M.I. Pravdin, I.E. Sleptsov, Astroparticle Physics **4**, 15 (1995)
145. A.V. Glushkov, L.G. Dedenko, M.I. Pravdin, I.E. Sleptsov, JETP **99,** 123 (2004).
146. A.V. Glushkov, S.V. Malinovskaya, Yu.G. Chernyakova, A.A. Svinarenko, Int. J. Quantum Chem. **99**, 889 (2004).

147. A.V. Glushkov, S.V. Malinovskaya, Int. J. Quantum Chem. 104, 496 (2005).
148. A. Glushkov, S. Malinvoskaya, O. Khetselius, Eur. Phys. J. ST **160**, 195 (2008).
149. A. Glushkov, S. Malinvoskaya, O. Khetselius, Mol. Phys. **106**, 1257 (2008).
150. A.V. Glushkov, O.Yu. Khetselius, S.V. Malinovskaya, in *Frontiers in Quantum Systems in Chemistry and Physics*, Series: *Progress in Theoretical Chemistry and Physics* , vol. 18, ed. by S.Wilson, P.J.Grout, J. Maruani, G. Delgado-Barrio, P. Piecuch (Springer, Berlin, 2008), pp. 523-540.
151. A.V. Glushkov, J. Appl.Spectr. (Springer) **74**, 305 (2007).
152. A.V. Glushkov, Sensor Electr. Microsyst. Techn. **3**, 21 (2006); **4**, 11

(2007); **5**, 41 (2008).
153. A.V. Glushkov, S.V. Ambrosov, A.V. Ignatenko, D.A. Korchevsky, Int. J. Quantum Chem. **99**, 936 (2004).
154. A.V. Glushkov, S.V. Malinovskaya, I.M. Shpinareva, V.P. Kozlovskaya, V.I. Gura, Int. J. Quantum Chem. **104**, 512 (2005).
155. Glushkov, A.V., Ambrosov, S.V., Loboda, A.V., Gurnitskaya, E.P., Prepelitsa, G.P. Int. J. Quantum Chem. **104**, 562 (2005).
156. A.V. Glushkov, A.V.Loboda, E.P. Gurnitskaya, A.A.Svinarenko, Phys. Scripta T **134**, 137740 (2009).
157. A.V. Glushkov, V.D. Rusov, S.V. Ambrosov, A.V. Loboda, in *New Projects and New Lines of Research in Nuclear Physics*, ed. by G. Fazio and F. Hanappe (World Scientific, Singapore, 2003), p. 126-142.
158. A.V. Glushkov, O.Yu. Khetselius, A.V.Loboda, A.A.Svinarenko, in *Frontiers in Quantum Systems in Chemistry and Physics*, Series: *Progress in Theoretical Chemistry and Physics*, vol. 18, ed. by S. Wilson, P.J. Grout., J. Maruani, G. Delgado-Barrio, P. Piecuch (Springer, Berlin, 2008), pp.541-588.
159. A.V. Glushkov, O.Yu. Khetselius, S.V.Malinovskaya, in *Frontiers in Quantum Systems in Chemistry and Physics*, Series: *Progress in Theoretical Chemistry and Physics*, vol. 18, ed. by S. Wilson, P.J. Grout., J. Maruani, G. Delgado-Barrio, P. Piecuch (Springer, Berlin, 2008), pp.523-540.
160. A.V. Glushkov, Spectral Line Shapes (AIP) **1092**, 258 (2010).
161. V.V.Tolmachev, Adv. Quant. Chem. **4**, 331 (1969).
162. V.S.Letokhov, Preprint of Physical Institute of the USSR Academy of Sciences (FIAN), N1-69 (FIAN. Moscow, 1969), pp.1-72.
163. V.S. Letokhov, Phys. Lett. A **46**, 257 (1974).
164. V.S. Letokhov, Laser Specktroskopie (Akad.-Verlag, Berlin, 1977).
165. V.I.Goldansky, V.S. Letokhov, Sov. Phys. JETP. **67**,513 (1974).
166. G.G.Baldwin, J.C.Salem, V.I.Goldansky, Rev.Mod.Phys. **53**, 687 (1981).
167. N.G.Basov, V.S.Letokhov, Sov.Phys.-Uspekhi. **11**, 855 (1969).
168. V.S. Letokhov, Science. **180** (N4085), 451 (1973).
169. V.S. Letokhov, L.N.Ivanov, Quantum Electronics (USSR) **2 (**N3), 585 (1975).
170. V.S. Letokhov, V.G.Minogin, B.D.Pavlik, Optics Comm. **19**, 72 (1976).

171. V.S. Letokhov, C.B.Moore, *Chemical and Biochemical Applications of Lasers*. (Acad.Press, New York, 1977), pp.1-670.
172. V.S. Letokhov, Nature, N**277**, 605 (22 February 1979).
173. V.S. Letokhov, in: *Apllication of Lasers in Atomic, Molecular and Nuclear Physics*, ed. by A.M.Prokhorov and V.S.Letokhov (Nauka, Moscow, 1979), pp.412-455.
174. V.S. Letokhov, V.I.Balykin, V.I.Mishin, G.I.Bekov, Sov.Phys.-Uspekhi. **132** (N10) 79 (1980).
175. V.S. Letokhov, *Nonlinear Selective Photo-processes in atoms and molecules* (Nauka, Moscow, 1983), pp.1-408.
176. V.S. Letokhov, V.G. Minogin, Sov.Phys.-Uspekhi. **147** (N9), 79 (1985).
177. V.S. Letokhov, Sov.Phys.-Uspekhi. **29**, 70 (1986); **41**, 523 (1998); **42**, 241 (1999).
178. V.S. Letokhov, V.I.Balykin, Sov.Phys.-Uspekhi. **33**, 79 (1990); Phys. Rev. A.**64**, 063410 (2001).
179. V.S. Letokhov, L.N.Ivanov, A.V.Glushkov, Preprint of Institute for Spectroscopy of USSR Academy of Sciences (ISAN), AS N5 (ISAN, Moscow-Troitsk, 1992), p.1-18.
180. N.G.Basov, E. Belenov, V.A.Isakov, E.A.Markin, Sov.Phys.-Uspekhi. **121**, 427 (1977).
181. V.S.Lisitsa, Sov.Phys.-Uspekhi. **153**, 379 (1977).
182. A.M.Prokhorov, N.V.Karlov, B.B.Krynetsky, V.A.Mishin, Sov.Phys.-Uspekhi. **137**, 593 (1979).
183. P.A. Bokhan, V.V.Buchanov, N.V.Fateev, M.M.Kalugin, M.A.Kazaryan, A.M.Prokhorov, D.E.Zakrevskii, *Laser Isotope Separation in Atomic Vapor* (Wiley-VCH, Berlin, 2006).
184. V.V.Buchanov, M.A.Kazaryan, M.Kalugin, A.M.Prokhorov, *Laser separation of Silicon Isotopes by the AVLIS Technology*, Series: *Atomic and Molecular Pulsed Lasers* (SO RAN, Tomsk, 2001).
185. W.Stoll, *Present Status of industrial Isotope separation by laser technology*, Series: *Atomic and Molecular Pulsed Lasers* (SO RAN, Tomsk, 2001).
186. F.J. Duarte, *Tunable Laser Optics* (Elsevier Academic, New York, 2003).
187. F.J. Duarte, Australian Physics. **47**, 38 (2010).

188. G.S., Janes, H.K., Forsen, R.H. Levy, The Exxon/Avco Program in Laser Enrichment: Uranium Enrichment; Research Report, N422 (Avco Everett Res. Lab., 1975).
189. S.Singh, K.Dasgupta, S.Kumar, K.Manohar, L.Nair, O. Chatterjee, Opt. Eng**. 33**, 1894 (1994).
190. R.W. Solarz, C.A.May, L.R.Carlson, E.F.Worden, S.A.Johnson, J.A.Paisner, L.J. Radziemski, Phys.Rev.A. **14**, 1129 (1976).
191. A.V. Glushkov, *Atom in an electromagnetic field* (KNT, Kiev, 2005), 450p.
192. Sokolovskaya, A.A. Soldatov, L.V. Chistyakov, JETP {94}, 1169--1178 (1984)

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CHAPTER 3. OPTIMIZED RELATIVISTIC MANY-BODY PERTURBATION THEORY IN CALCULATIONS OF ENERGY AND SPECTRAL CHARACTERISTICS OF RELATIVISTIC ATOMS AND MULTICHARGED IONS

3.1 Introduction

In this chapter the radiative transitions wavelengths and oscillator strengths for some Li-like multicharged ions are calculated within the relativistic many-body perturbation theory with the optimized Dirac-Kohn-Sham zeroth approximation and an effective taking the relativistic, exchange-correlation, nuclear, radiative effects into account. There have been considered all correlation corrections of the second order and dominated classes of the higher orders diagrams (3.electrons screening, mass operator iterations etc). The method includes the generalized Glushkov-Ivanov-Ivanova procedure (3.relativistic energy approach) for generation of the optimal basis set of relativistic electron wave functions with fulfilment of the gauge invariance principle. To reach the latter we focus on accurate consideration of the QED perturbation theory fourth order (3.a second order of the atomic perturbation theory) Feynman diagrams, whose contribution into imaginary part of radiation width Im δE for the multi-electron ions accounts for multi-body correlation effects. A minimization of the functional ImδE leads to integral-differential Dirac-Kohn-Sham-like density functional equations. The magnetic inter-electron interaction is accounted for in the lowest order on α^2 (3.α is the fine structure constant) parameter. The Lamb shift polarization part is taken into account in the modified Uehling-Serber approximation. Comparisons of our results on the radiative transition wavelengths and oscillator strengths for some transition in spectra of the Li-like multicharged ions (3.the nuclear charge Z=21-30) with other comparable

The study of spectroscopic and structural properties of the multicharged ions has a subject of significant interest for many physical, astrophysical and chemical applications. The levels energies, transitions probabilities, oscillator strengths and so on are very important in atomic physics (3.spectroscopy, spectral lines theory), astrophysics, plasma physics, laser physics, quantum electronics. They are very much needed in research of thermonuclear reactions, where

the ionic radiation is one of the primary loss mechanisms and so on. The spectral lines belonging to the radiation of many multicharged ions have been identified in both solar flares and nonflaring solar active regions, observed in high-temperature plasmas, such as pinches and laser-produced plasmas, and in beam-foil spectra. The multiple observations of satellite lines of the He-, Li-, Be-like multicharged ions in the solar corona and in laboratory plasmas have emphasized the need for accurate values of the energetic and spectroscopic parameters for multicharged ions. The experiments on the definition of hyperfine splitting also enable to refine the deduction of nuclear magnetic moments of different isotopes and to check an accuracy of the various computational models employed for the theoretical description of the nuclear effects. Generally speaking, studying the spectra, radiative transition oscillator strengths, hyperfine structure parameters and so on for heavy elements and multicharged ions is of a great significance for the further development of atomic and nuclear theories and spectroscopy of multicharged ions (3.see, for example, Refs. [1-120]). To obtain an accurate transition oscillator strengths, hyperfine structure parameters and so on, accurate wave functions must be used for both the initial and finial states.

The accurate calculation of energetic and spectroscopic properties for the multicharged ions over the past decades has been driven primarily by the steady development of quantum theory, on the one hand, and increasing computing power, on the other hand. As a rule, the most accurate calculations have been performed for the simple, few-electron atomic systems, such as the helium atom and its isoelectronic ions. Newly developed quantum approaches as well as advanced traditional quantum chemical methods have been approbated on few-electron atomic systems. Theoretical calculations have concentrated mainly on obtaining accurate transition wavelengths and oscillator strengths which are necessary for multiple applications. On the other hand, these calculations made it possible to check the quality and accuracy of the atomic wave functions.

Many theoretical methods including multiconfiguration Hartree–Fock (3.HF) method (3.for example, by Sundholm, Olsen and Fischer et al), configuration-interaction methods, multiconfiguration Dirac–Fock (3.DF), many-body perturbation theory (3.MBPT) and its relativistic MBPT version (3.RMBPT) (3.in particular, by Lindgren and coworkers), method of variational wave function in the Hylleraas coordinates and so on (3.see [9-59] and Refs. therein) have

been developed for accurate calculations of spectroscopic characteristics of few-electron atoms and multi-charged ions.

Let us mention the extended optimal level (3.EOL) version of the MCDF method, which was used to calculate the transitions in the GRASPVU program package. The multi-configuration relativistic HF and DF approaches are the most reliable versions of calculation for multi-electron systems with a large nuclear charge. Usually, in these calculations the one- and two-body relativistic effects are taken into account practically precisely. Special attention should be given to three very general and important computer systems for relativistic and QED calculations of atomic and molecular properties developed by Oxford and German-Russian groups etc (3.“GRASP”, “Dirac”; “BERTHA”, “QED”, “Dirac”) (3.see [9-59] and Refs. therein). For example, the BERTHA program embodies a new formulation of relativistic atomic and molecular structure theory within the framework of relativistic quantum electrodynamics (3.QED). This leads to a simple and transparent formulation of the Dirac-Hartree-Fock-Breit self-consistent field equations along with algorithms for molecular properties, electron correlation, and higher order QED effects.

These equations are solved by a direct method based on a relativistic generalization of the McMurchie-Davidson algorithm for corresponding integrals that economizes memory requirements and is not significantly more expensive computationally than comparable nonrelativistic calculations. The useful overview of the relativistic electronic structure theory is presented in refs. [23,24,109-120] from the QED point of view. The next important step is an adequate taking into account the QED corrections. This topic has been a subject of intensive theoretical and experimental interest (3.see, for example, [81-97]).

In many calculations of characteristics of the atomic elementary processes it has been shown that an adequate description of these characteristics requires using the optimized wave functions in order to provide obtaining more accurate spectral data and simultaneously solving the convergence problems, for example, in the method of configurational interaction or any version of the atomic or molecular perturbation theories [1-22,117-152]. We would like to mention that one of the first most effective attempts to construct optimal one-quasiparticle representation in quantum chemistry belonged to outstanding Swedish scientist Per-Olov Löwdin in 1955 (3.see, c.g., [1-4]). He introduced the concept

of *natural orbitals* to describe the unique set of orthonormal one-electron functions that are intrinsic to the *N*-electron wave function.

Subsequently many scientists, including Davidson et al [6,15,16], pointed the principal disadvantages of the traditional representation based on the self-consistent field approach and suggested the optimal "natural orbitals" representation.

Davidson et al have introduced the frozen natural orbital approach. The main advantage here is that the state vectors are obtained much "cleaner" than in the self-consistent field representation, which simplifies the actual calculation of the energy matrix and matrix elements of other operators. Nevertheless, there remain insurmountable calculational difficulties in the full realization of the Davidson program.

In the last years new ideas to problem of optimal representation were proposed (3.see details in Refs.[1-22]). A great interest attracts an advanced frozen natural orbital concept for ionized states within equation of motion-coupled clusted approach. It is necessary to note that one of the simplified recipes is the Kohn-Sham density functional method [13,14]. Unfortunately, this method doesn't provide a full regular refinement procedure in a case of the complicated atomic systems with several quasiparticles (3.electrons or vacancies above a core of the closed electron shells), though a significant progress is achived in the last years. Some alternative recipes for construction of the optimal one-quasiparticle representation are presented in a series of papers [51-64,69-71].

One of the most exotic approaches to construction of the optimal one-quasiparticle representation includes variation of the gauge constant of electromagnetic interaction as adjusting (3.fitting) parameter (3.see, c.g. [28]). In our opinion, one of the most consistent and effective methods to obtain the optimal represantation was developed by Glushkov-Ivanov [127] within relativistic energy approach combined with the RMBPT (3.or QED PT). They proposed the fundamental optimization principle, related to the minimization of the density functional, which is the contribution of the QED PT fourth-order polarization Feynman diagrams (3.or atomic PT second order). For example, while treating the one-quasiparticle atomic systems (3.one electron above or vacancy in the closed electron shells core) the contribution of these diagrams is

determined by the polarization of the core by the quasi-quasiparticle [127-136]. These are the first diagrams in which collective effects manifest themselves and their contributions depend on the calibration of the potentials of the electromagnetic field (3.gauge-noninvariant contributions). The authors [127] calculated the contribution of the polarization diagrams associated with the exchange of longitudinal photons in the imaginary part of the energy of the excited state. However, the total numerical minimization of the gauge-noninvariant contribution has not been performed. There was presented a more simplified model, based on variation of the Ivanov-Ivanova model potential [119,124,132,134] parameter to provide the gauge-noninvariant contribution minimization.

In this chapter for the first time we present the full consistent realization of the Glushkov-Ivanov approach within our version of the RMBPT with the optimized Dirac-Kohn-Sham (3.DKS) zeroth approximation and apply it to computing the levels energies, oscillator strengths of a number of the radiative transitions, hyperfine structure parameters for the Li-like multicharged ions. The method used is designed for calculations of multi-electron atomic systems with accounting for the relativistic, correlation, nuclear, radiative effects. All correlation corrections of the second order and dominated classes of the higher orders diagrams (3.electrons screening, mass operator iterations etc.) have been taken into account [93-102]. The magnetic inter-electron interaction is accounted for in the lowest order on α^2 parameter. The Lamb shift polarization part is taken into account in the modified Uehling-Serber approximation. The Lamb shift self-energy part is accounted for effectively within the generalized Ivanov-Ivanova non-perturbative procedure [121,122]. Comparisons of our results with other comparable calculations and with the experimental results will also be given and discussed.

There have been sufficiently many reports of theoretical and experimental studies of energies and oscillator strengths for the Li-like ions and other alkali-like ions (3.see, for example, [29–63]). Aglitskii et al [121] experimentally observed the Lα wavelengths of Li-like ions (3.Z = 19–26) in laser-produced plasmas. Theoretical approach to studying the spectroscopic characteristics of the heavy multicharged ions (3.Li-like ions) within the RMBPT with the model potential zeroth approximation is developed by Ivanov-Ivanova [119-125]. Banglin Deng

et al [52] presented the calculated wavelengths, oscillator strengths, transition probabilities, and line strengths for Li-like ions (3.Z = 7–30) in the framework of the relativistic configuration-interaction formalism using MCDF wave functions and considering the Breit interaction, QED and nuclear mass corrections. A critical evaluation and compilation of the spectroscopic parameters for Li-like ions (3.*Z*=3-28) was undertaken by Martin and Wiese [153-156]. Bièmont [30] applied fully variational nonrelativistic HF wave functions in computing 1s2n2L (3.n<8=s,p,d,f; 3<*Z*<22) Li-like states].

Chen Chao and Wang Zhi-Wen [48] applied a full core plus correlation method with using multiconfiguration interaction wave functions to computing the nonrelativistic values of the oscillator strengths for a number of transitions into the Rydbers states along the LiI isoelectronic sequence. The Hylleraas-type variational method and the 1/*Z* expansion method have been used also to obtain the non-relativistic calculations data on the energies and oscillator strengths of 1*s*22*s*,1*s*22*p* for Li-like systems up to *Z* = 50 [41-51]. Fully relativistic computing the wavelengths and oscillator strengths from excitation of Li-like ions (3.*Z* = 8–92) have been given by Zhang et al. [53]. Nahar [54] applied the Breit–Pauli R-matrix method to calculations of the wavelengths, transition probabilities, and oscillator strengths for a number of the Li-like ions with the nuclear charge *Z*=6-68. The relativistic quantum defect method has been used by Martin et al [55] to calculate the oscillator strengths for a number of radiative transitions between low-lying states in the Li-like ions for Z < 45. The energy levels and hyperfine constants of neutral lithium were studied by Lindgren[9] within a nonrelativistic coupled-cluster method, by Guan-Wang [47] within the effective operator form of MBPT etc. Relativistic all-order MBPT calculations of energies and matrix elements for Li and Be+ were reported in Ref. [44]. Wu Xiao-Li et al [50] have performed the relativistic MBPT calculation for lithium-like isoelectronic sequence (3.*Z*=3−9) within the DF method with using the finite basis sets of the Dirac–Fock equations, constructed by B splines. Consistent QED treatment of the levels energies, fine structure etc is presented by the Notre-Dame and St. Petersburg groups [37,111,112, 115]. Despite a great number of fulfilled works on the lithium and Li-like ions, at the present time the systematic studies of the wavelengths, radiative rates, oscillator strengths, hyperfine parameters for the

Li-like multicharged ions are still needed for the multiple applications, future experiments etc.

3.2. Relativistic many-body perturbation theory with the Dirac-Kohn-Sham zeroth approximation

3. 2.1. The Dirac-Kohn-Sham zeroth approximation and nuclear potential.

The theoretical basis of the RMBPT with the Dirac-Kohn-Sham zeroth approximation was widely discussed [26,27,93-102], and here we will only present the essential features. We will focus on more detailed presentation of the procedure for construction of an optimal quasiparticle representation within our version of the RMBPT. The electron wave functions (3.the PT zeroth basis) in our method are naturally found from solution of the relativistic Dirac equation with potential, which includes ab initio mean-field DKS potential, electric, polarization potentials of a nucleus. The charge distribution in the Li-like ion is modelled within the Gauss model, though the alternative nuclear models such as the Fermi one, or the independent particle model with the Woods-Saxon and spin-orbit potentials, and relativistic mean-field theory were earlier used too.

We set the charge distribution in the Li-like ion nucleus $\rho(3.r)$ by the Gaussian function:

$$\rho(r|R) = \left(4\gamma^{3/2}/\sqrt{\pi}\right)\exp\left(-\gamma r^2\right) \qquad (3.1)$$

where $\gamma=4/\pi R^2$ and R is the effective nucleus radius. The Coulomb potential for the spherically symmetric density $\rho(3.\ r\ )$ is:

$$V_{nucl}(r|R) = -\left((1/r)\int_0^r dr'\,r'^2\rho\left(r'\middle|R\right) + \int_r^\infty dr'\,r'\rho\left(r'\middle|R\right)\right) \qquad (3.2)$$

In order to determine the nuclear potential we apply the known method of differential equations by Ivanova-Ivanov [119,122]. Calculation of potential (3.2) reduces to solving the following system of differential equations:

$$V'_{nucl}(r,R)=\left(1/r^2\right)\int_0^r dr' r'^2 \rho\left(r',R\right)\equiv\left(1/r^2\right)y(r,R) \qquad (3.3a)$$

$$y'(r,R)=r^2\rho(r,R) \qquad (3.3b)$$

$$\rho'(r,R)=-8\gamma^{5/2}\, r/\sqrt{\pi}\exp\left(-\gamma r^2\right)=-2\gamma r\rho(r,R)=-\frac{8r}{\pi r^2}\rho(r,R) \qquad (3.3c)$$

with the corresponding boundary conditions.
The corresponding derivative of potential on the nuclear radius is as follows:

$$\partial W\left(r|R\right)/\partial r = W(r)\int_0^r dr\, r^2 \partial\rho\left(r|R\right)/\partial R+\int_0^\infty dr\, r^2 W(r)\partial\rho\left(r|R\right)/\partial r \ . \qquad (3.4)$$

The derivative of the physical characteristics, corresponding to potential $W(r|R)$, on the nuclear radius is represented by the matrix element:

$$\partial W(R)/\partial R=\int_0^\infty dr\, r^2\left[F^2_{nlj}(r)+G^2_{nlj}(r)\right]\partial W\left(r|R\right)/\partial R \qquad (3.5)$$

As a rule, the nuclear finite size correction is not correctly taken into account within the perturbation theory as a matrix element of two potentials difference. It is well known that the functions of a state for two nuclear potentials differ significantly in the important region. Calculation of the potentials, their derivatives, matrix elements is reduced to solving the single system (3.in fact 1D procedure) of differential equations [28,29,119,135]. For example, in order to calculate the potentials *W (3.r|R)* and *∂W(3.r|R)/∂R* the following system of differential equations should be solved:

$$dW(3.r|R)/dr=P(3.r|R)dW(3.r)/\,dr\ ,$$

$$dP\ (3.r|R)=r^2\rho(3.r|R)\ ,$$

$$d[\partial W(3.r|R)/\partial R\ ]/dr=S(3.r|R)dW(3.\ r)/dr\ ,$$

$$dS(3.r|R)/dr=r^2[\partial\rho(3.r|R)/\partial R\ ] \qquad (3.6)$$

with known analytical functions *W(3.r), ρ (3.r|R)*. The boundary values at $r \to 0$ are found by expansion to a set on r.

Further consider the DF type equations for a three-electron system $1s^2nlj$. As usually, the differential equations for the radial functions *F* and *G* (3.components of the Dirac spinor) are as follows: :

$$\frac{\partial F}{\partial r}+(1+\chi)\frac{F}{r}-(\varepsilon+m-V)G=0,$$
$$\frac{\partial G}{\partial r}+(1-\chi)\frac{G}{r}+(\varepsilon-m-V)F=0, \qquad (3.7)$$

where *F*, *G* are the large and small components respectively; the fine structure constant α=1; χ is the quantum moment number.

At large χ, the functions *F* and *G* vary rapidly at the origin; we have:

$$F(r),G(r)\approx r^{\gamma-1}, \qquad (3.8a)$$

$$\gamma=\sqrt{\chi^2-\alpha^2 z^2} \qquad (3.8b)$$

This creates difficulties in numerical integration of the equations in the region $r\to 0$. To prevent the integration step from becoming too small it is usually convenient to turn to new functions isolating the main power dependence: $f = Fr^{1-|\chi|}$, $g = Gr^{1-|\chi|}$. The Dirac equations for *F* and *G* components are transformed as follows (3.in the Coulomb units):

$$f' = -(\chi+|\chi|)f/r-\alpha ZVg-(\alpha ZE_{n\chi}+2/\alpha Z)g, \qquad (3.9a)$$

$$g' = (\chi-|\chi|)g/r-\alpha ZVf+\alpha ZE_{n\chi}f. \qquad (3.9b)$$

Here $E_{n\chi}$ is one-electron energy without the rest energy. The boundary values are defined by the first terms of the Taylor expansion:

$$g=\left(V(0)-E_{n\chi}\right)r\alpha Z/(2\chi+1);\quad f=1 \text{ at } \chi<0,$$

$$f=\left(V(0)-E_{n\chi}-2/\alpha^2Z^2\right)\alpha Z;\quad g=1 \text{ at } \chi>0. \qquad (3.9b)$$

The condition f, $g\to 0$ at $r\to\infty$ determines the quantified energies of the state $E_{n\chi}$.

Formally a potential $V(3.r|R)$ in Eqs. (3.8) includes-electric and polarization potentials of the nucleus, V_X is the exchange inter-electron interaction (3.in the zeroth approximation). The standard Kohn-Sham (3.KS) exchange potential is [13]:

$$V_X^{KS}(r)=-(1/\pi)[3\pi^2\rho(r)]^{1/3}. \qquad (3.10)$$

In the local density approximation the relativistic potential is [33]:

$$V_X[\rho(r),r]=\frac{\delta E_X[\rho(r)]}{\delta\rho(r)}, \qquad (3.11)$$

where $E_X[\rho(r)]$ is the exchange energy of the multielectron system corresponding to the homogeneous density $\rho(r)$, which is obtained from a Hamiltonian having a transverse vector potential describing the photons. In this theory the exchange potential is [33]:

$$V_X[\rho(r),r]=V_X^{KS}(r)\cdot\{\frac{3}{2}\ln\frac{[\beta+(\beta^2+1)^{1/2}]}{\beta(\beta^2+1)^{1/2}}-\frac{1}{2}\}, \qquad (3.12)$$

where $\beta=[3\pi^2\rho(r)]^{1/3}/c$, c is the velocity of light. The corresponding one-quasiparticle correlation potential

$$V_C[\rho(r),r]=-0.0333\cdot b\cdot\ln[1+18.3768\cdot\rho(r)^{1/3}], \qquad (3.13)$$

(3.here b is the optimization parameter; see below).

The perturbation operator contains the relativistic potential of the interelectron interaction of the form:

$$V_{e-e}^{rel}(r_i, r_j) = \frac{\left(1 - \alpha_i \alpha_j\right)}{r_{ij}} \exp(i\omega_{ij} r_{ij}), \qquad (3.14)$$

(3.here α_i ,α_j are the Dirac matrices, ω_{ij} is the transition frequency) with the subsequent subtraction of the exchange and correlation potentials. The rest of the exchange and correlation effects will be taken into account in the first two orders of the PT [93-102].

3.2.2. QED corrections.

A procedure of taking into account the radiative QED corrections is in details given in the refs. [11,14,20-22]. Regarding the vacuum polarization effect let us note that this effect is usually taken into consideration in the first PT theory order by means of the Uehling-Serber potential. This potential is usually written as follows:

$$U(r) = -\frac{2\alpha}{3\pi r} \int_1^\infty dt \exp\left(-2rt/\alpha Z\right)\left(1 + 1/2t^2\right)\frac{\sqrt{t^2 - 1}}{t^2} \equiv -\frac{2\alpha}{3\pi r} C(g), \qquad (3.15)$$

where $g=r/(3.\alpha Z)$. In our calculation we use more exact approach [93]. The Uehling-Serber potential, determined as a quadrature (3.6), may be approximated with high precision by a simple analytical function. The use of new approximation of the Uehling-Serber potential permits one to decrease the calculation errors for this term down to 0.5 – 1%. A method for calculation of the self-energy part of the Lamb shift is based on an idea by Ivanov-Ivanova [119,121]). In an atomic system the radiative shift and the relativistic part of energy are, in principle, defined by one and the same physical field. It may be supposed that there exists some universal function that connects the self -energy correction and the relativistic energy. The self-energy correction for the states of a hydrogen-like ion was presented by Mohr [109]:

$$E_{SE}(H|Z,nlj) = 0.027148\,\frac{Z^4}{n^3}\,F(H|Z,nlj) \qquad (3.16a)$$

These results are modified here for the states $1s^2$ *nlj* of Li-like ions. It is supposed that for any ion with *nlj* electron over the core of closed shells the sought value may be presented in the form [121]:

$$E_{SE}(Z,nlj) = 0.027148\,\frac{\xi^4}{n^3}\,f(\xi,nlj)\left(cm^{-1}\right) \qquad (3.16b)$$

The parameter $\xi=(3.E_R)^{1/4}$, E_R is the relativistic part of the bounding energy of the outer electron; the universal function $f(\xi,nlj)$ does not depend on the composition of the closed shells and the actual potential of the nucleus. The procedure of generalization for a case of Li-like ions with a finite nucleus consists of the following steps: i). calculation of the values E_R and ξ for the states *nlj* of H-like ions with the point nucleus (3.in accordance with the Sommerfeld formula); ii). construction of an approximating function $f(\xi,nlj)$ by the found reference *Z* and the appropriate $F(H|Z,nlj)$;

iii). calculation of E_R and ξ for the states *nlj* of *Li*-like ions with a finite nucleus; iv). calculation of E_{SE} for the sought states by the formula (3.43). The energies of the states of Li-like ions were calculated twice: with a conventional constant of the fine structure α=1/137.03597 and with $\tilde{\alpha} = \alpha/1000$. The results of latter calculations were considered as non-relativistic. This permitted isolation of E_R and ξ. A detailed evaluation of their accuracy may be made only after a complete calculation of $E^n_{SE}(Li\,Z,nlj)$. It may be stated that the above extrapolation method is more justified than using the widely spread expansions by the parameter αZ.

3.3. Construction of the optimal one-quasi-electron representation

In Ref. [127,128] it has been proposed “ab initio” optimization principle for construction of the optimal relativistic orbital basis set. The minimization condition of the gauge dependent multielectron contribution of the lowest QED

PT corrections to the radiation widths of the atomic levels is used. The details of procedure can be found in Ref. [126-134].

As in Ref. [127, 134], let us examine the multi-electron atomic ion with one quasiparticle in the first excited state, connected with the ground state by the electric dipole radiation transition. In the QED PT zeroth order we use the one-electron bare potential $V_N(3.r)+V_X(3.r)+ V_C(3.r)$. As usual, the perturbation operator is as follows:

$$-V_{Xc}(r) - J_{\mu}(x) A^{\mu}(x) \qquad (3.17)$$

где A — vector-potential of the electromagnetic field, J — current operator. Figure 1a presents a single B diagram of the second order PT, which contributes to the imaginary part of the energy shift (3.or the radiation width of the atomic level) ImδE. In the fourth order of QED PT, the sought diagrams are A_d (3.direct polarization diagram, Fig. 1b) и A_{ex} (3.exchange polarization diagram, Fig. 1c), describing the effect of polarization of closed electronic shells. Further, using the standard S-matrix technique, the contributions to the value ImδE, corresponding to the various diagrams in Fig. 2.2, are calculated. The electron propagator is presented in a standard form.

. We recall that each electronic line of the diagram is associated with an electron propagator:

$$\begin{aligned} G(X_1, X_2) &= -\sum_{s\le f} \exp(-i\omega_s t_{12})\psi_s(r_1)\psi_s^{+}(r_2), t_1 < t_2 \\ G(X_1, X_2) &= \sum_{s> f} \exp(-i\omega_s t_{12})\psi_s(r_1)\psi_s^{+}(r_2), t_1 > t_2 \end{aligned} \qquad (3.18)$$

The operator ψ_s^{+} corresponds to the terminal electronic line entering the diagram and ψ_s - outgoing line; $\sum_{\substack{n>f \\ m\le f}}(...)$ denotes summation over all electronic states above (3.below) the Fermi level of electrons in the core, including the upper continuum. Each dotted line corresponds to the expression: $\gamma^{\mu} D_{\mu\nu} \gamma^{\nu}$. The form of a photon propagator $D_{\mu\nu}$, naturally, is determined by its gauge. For the commonly used Coulomb gauge:

$$D_{\mu\nu} = -\frac{1}{8\pi^2}\delta_{\mu\nu}\frac{1}{r_{12}}\int d\omega \exp\left(-i\omega t_{12} + i|\omega|r_{12}\right) \qquad (3.19a)$$

After integrating by times the dashed line corresponds to the "operator" of the interelectron interaction:

$$\frac{e^2}{4\pi}\frac{1}{r}\exp(i|\omega|r_{12})(1-\alpha_1\alpha_2) \qquad (3.19b)$$

According to [127], contribution to ImδE of B diagram is represented as follows:

$$\mathrm{Im}\,\delta E_\alpha(B_1) = \sum \mathrm{Im}\,\delta E(\alpha - s\,|B_1) \qquad (3.20)$$

Expression (3.20) is the sum of the partial contributions of the transitions from the initial state | α > to the final state | s> (3.the levels α and s are connected by an electrically dipole radiative transition). In general, the calibration of the photon propagator can be written in the following standard form:

$$D = D_T + C \cdot D_L \qquad (3.21a)$$

$$D_T = \frac{\delta_{\mu\nu}}{k_0^2 - k^2}, \qquad (3.21b)$$

$$D_L = \frac{k_\mu k_\nu}{k_0^2 - k^2}, \qquad (3.21c)$$

where D_T represents the electron exchange by transverse photons, D_L — by longitudinal photons, and C is the gauge constant.

The contribution of the second-order diagram to the partial radiation width of the level α is equal under condition $D=D_T$ (3.see Refs.[127,128]):

$$-\frac{e^2}{8\pi}\iint dr_1 dr_2 \psi_\alpha^+(r_1)\psi_s^+(r_2)D_T(r_1 r_2)\psi_\alpha(r_2)\psi_s(r_1) \qquad (3.22a)$$

Similarly, for $D=D_L$ the contribution of the second-order diagram to the partial radiation width of the level α is equal to:

$$-\frac{e^2}{8\pi}\iint dr_1 dr_2 \psi_\alpha^+(r_1)\psi_s^+(r_2)D_L(r_1 r_2)\psi_\alpha(r_2)\psi_s(r_1) \qquad (3.22b)$$

where

$$D_T(r_1 r_2) = (1-\alpha_1\alpha_2)\sin\omega_{\alpha s} r_{12}/r_{12} \qquad (3.22c)$$

$$D_L(r_1 r_2) = [1-(\alpha_1 n_{12})(\alpha_2 n_{12})]\sin\omega_{\alpha s} r_{12} + \\ +\omega_{\alpha s}[1+(\alpha_1 n_{12})(\alpha_2 n_{12})]\cos\omega_{\alpha s} r_{12} \qquad (3.22d)$$

It should be recalled that, in view of Grant's well-known theorem, if electronic wave functions of the atom Ψ_α, Ψ_s satisfy the same Dirac equation, then the contribution $D_{\mu\nu}$,, is equal to 0.

Further one may treat the lowest order multi-electron effects, in particular, the gauge dependent radiative contribution for a certain class of the photon propagator calibration. The contribution of the QED PT fourth order diagrams A (3.Fig.1b,1c) into the ImδE accounts for the exchange-polarization effects. In fact it describes the collective effects and is dependent upon the electromagnetic potentials gauge (3.the gauge non-invariant contribution). This value is considered to the typical electron correlation effect, whose minimization is a reasonable criterion in searching the optimal one-electron basis of PT. All the gauge non-invariant terms are multi-electron by their nature (3.the particular case of the gauge non-invariance manifestation is the non-coincidence of the oscillator strengths values, obtained in the approximate calculations with the "length" and "velocity" transition operator forms). Quite complicated calculation of contribution of the QED PT fourth order polarization diagrams into Im δE gives the following result [127]:

$$\mathrm{Im}\delta E_{ninv}(\alpha - s;b) = -C\int\int\int\int dr_1 dr_2 dr_3 dr_4 \sum_{\substack{n>f \\ m\le f}} \left(\frac{1}{\omega_{mn} + \omega_{\alpha s}} + \frac{1}{\omega_{mn} - \omega_{\alpha s}} \right) \cdot \cdot$$

$$\cdot \psi_\alpha{}^+(r_1)\psi_m{}^+(r_2)\psi_s{}^+(r_4)\psi_n{}^+(r_3)\frac{1-\alpha_1\alpha_2}{r_{12}}\{[(\alpha_3\alpha_4 - \alpha_3 n_{34}\alpha_4 n_{34})/r_{14}]\cdot$$

$$\cdot sin[\omega_{\alpha n}(r_{12}+r_{34})] + \omega_{\alpha n} cos[\omega_{\alpha n}(r_{12}+r_{34})](1+\alpha_3 n_{34}\alpha_4 n_{34})\}\cdot$$

$$\cdot \psi_m(r_3)\psi_\alpha(r_4)\psi_n(r_2)\psi_s(r_1). \qquad (3.23)$$

Here, f is the boundary of the closed shells; $n \ge f$ indicates the unoccupied bound and the upper continuum electron states; $m \le f$ indicates the finite number of states in the core and the states of the negative continuum (3.accounting for the electron vacuum polarization). The expression (3.23) can be represented in the form of terms:

$$\sum_{\substack{n>f \\ m\le f}} < \alpha m | W_1 | ns >< sn | W_2 | m\alpha > /(\omega_{mn} \pm \omega_{\alpha s}) \qquad (3.24)$$

with four different combinations of operators W_1 and W_2 (3.see details in Refs. [127-129]). The sum over n can be calculated by the method of differential equations. The index m numbers a finite number of states occupied in the core and the state of the real continuum. The continuum-related part describes the vacuum polarization of the electron field and leads to divergent integrals in the non-renormalizable theory. Its contribution to the main contribution has an additional order of smallness (3.αZ^2).

The minimization of the density functional ImδE leads to the integral differential equation for the ρ_c, that can be numerically solved. This step allows to determine the optimization parameter b. In Ref. [127] the authors elaborated a simplified computational procedure. Here for the first time we present the full consistent realization of the optimization approach within our version of the RMBPT. The procedure of minimization of the functional ImδE_{ninv} is fulfilled under the condition:

$$\int dr\, r^2\, \rho_c(r) = 1 \qquad (3.25)$$

and is reduced to a chain of the following variations:

$$\delta\rho_c \to \delta V_c \to \delta\{f_\alpha, f_s, g_\alpha, g_s\} \to \delta X,$$

$$\delta Y \to \delta Y_i \to \delta Z_i \to \delta I \to \delta E. \qquad (3.26)$$

Here f and g are the large and small components of the Dirac function $\psi_s(r)$ which are solutions of the relativistic DKS equation with potential

$$V_{\mathrm{N}}(r) + V_{\mathrm{C}}(r) + V_{\mathrm{X}}(r) + V_{\mathrm{cor}}(r).$$

The first link of the chain of variations is realized with the is performed help of:

$$\delta V_C = \frac{1}{r}\int_0^r dr' r'^2\, \delta\rho_c(r') + \int_0^\infty dr' r' \rho_c(r') \qquad (3.27a)$$

or

$$\delta V_C(r) = \frac{1}{r}\int_0^r dr' r'^2\, \delta\rho_c(r') + \int_r^\infty dr' r' \delta\rho_c(r') + X_1 \delta\rho_c(r)\{\frac{3}{2}\ln\frac{[\beta+(\beta^2+1)^{1/2}]}{\beta(\beta^2+1)^{1/2}} - \frac{1}{2}\} / \rho_c^{2/3}(r) +$$

$$+ ... + X_2 \delta\rho_c(r)\{\frac{3}{2}\ln\frac{[\beta+(\beta^2+1)^{1/2}]}{\beta(\beta^2+1)^{1/2}} - \frac{1}{2}\} / [(1+18.3768\cdot\rho_c(r)^{1/3})\rho_c^{2/3}(r)] + ..., \qquad (3.27b)$$

Here X_1 and X_2 - numerical coefficients. On the next stage we calculate a first-order correction by δV_{C} for the functions f_α, f_s, g_α, g_s - solutions of the DKS equation with the total one-particle potential, which is actually a bispinor of the form [13]:

$$\Phi_{\mu m} = \sum_{n_i} \Psi_{n_i\mu_i m_i} \langle n_i\mu_i m_i|V|n\mu m\rangle / (\varepsilon_{n_i\mu_i m_i} - \varepsilon) \qquad (3.28)$$

where $(3.n\mu m)$ – quantum numbers of one-electron states, ε - energy parameter. The corresponding components of the bispinor (3.28) satisfy the Dirac type system of equations by Glushkov-Ivanov-Ivanova [127] with more complicated view, namely:

$$-F'/\alpha Z + (1+\mu_i)F/\alpha Zr + A\_G = \delta V_C g_{n_i\mu_i}, \tag{3.29a}$$

$$G'/\alpha Z + (1-\mu_i)G/\alpha Zr + A_+F = \delta V_C f_{n_i\mu_i}, \tag{3.29b}$$

where functions $A_\pm$ are defined by expressions:

$$A_\pm = V_C(r) \pm 1/(\alpha Z)^2 - \varepsilon. \tag{3.30}$$

Solutions of system (3.29) are represented in the form of quadratures and contain pairs of the fundamental solutions (3.29) without right-hand sides.
The functions X and Y (3.26) are bilinear combinations of radial functions:

$$\{X,Y\} = \{f_\alpha f_s r^t; g_\alpha g_s r^t; f_\alpha g_s r^u; g_\alpha f_s r^u\}, \tag{3.31}$$

and their variations are calculated elementary. The contribution (3.24) is determined by the sum of radial integrals of the type:

$$I = \iiint dr_1 dr_2 dr_3 X(r_1)Y(r_2)Z(r_3)L(r_1r_3)M(r_2r_3) \tag{3.32a}$$

where

$$\{L_1, M_1\} = Z_\lambda^{(1)} r^p, \tag{3.32b}$$

$$\{L_2, M_2\} = Z_\lambda^{(2)} r^q, \tag{3.32c}$$

$$Z(r) = \rho_C^{1/3}(r) r^{\nu}, \qquad (3.32d)$$

Here $z_{\lambda}^{(1)}$, $z_{\lambda}^{(2)}$ are the reduced Bessel functions, λ=0,1; p,q,t,u,v are some integers;

The complete expression for δE contains a set of radial integrals of the type (3.32a) with rather cumbersome angular coefficients containing 6-j Wigner symbols (3.Racah W-coefficients) and 9-j symbols of Fano. The calculation of the functions Z and Y and their variations is reduced to a numerical solution of the system of differential equations, for which the standard Runge-Kutta numerical procedure of the fourth order (the 'Superatom-ISAN' computational code) is used.

So, the implementation of the minimization principle results in a system of integral differential equations, and its solution gives the optimal one-quasiparticle representation. The system is rather cumbersome and is solved with the help of our computational code.

3.4. Relativistic energy approach to computing oscillator strengths for multicharged ions.

Here we briefly present the key elements of the relativistic energy approach to computing radiation widths and oscillator strengths for atomic systems. Let us remind that an initial general energy formalism combined with an empirical model potential method in a theory of atoms and multicharged ions has been developed by Ivanov-Ivanova et al [119-125], further more general ab initio gauge-invariant relativistic approach has been presented in [127,128]. We use the optimized version of this formalism with our construction of one-quasiparticle representation. In the energy approach [124-126] the imaginary part of electron energy shift of an atom is connected with the radiation decay possibility (3.transition probability). An approach, based on the Gell-Mann and Low formula with the QED scattering matrix, is used in treatment of the relativistic atom. The total energy shift of the state is usually presented in the form:

$$\delta E = \mathrm{Re}\,\delta E + \mathrm{i}\Gamma/2 \qquad (3.33)$$

where Γ is interpreted as the level width, and the decay probability

$$P = \Gamma.$$

For the α-s radiation transition the imaginary part of electron energy in the lowest order of perturbation theory is determined as [124]:

$$\mathrm{Im}\,\delta E = -\frac{1}{4\pi}\sum_{\substack{\alpha>n>f\\ [\alpha<n\le f]}} V_{\alpha n\alpha n}^{|\omega_{\alpha n}|}, \qquad (3.34)$$

where $\omega_{\alpha n}$ is a frequency of the α-n radiation, (3.α>n>f) for electron and (3.α<n<f)
for vacancy.
The matrix element V is determined as follows:

$$V_{ijkl}^{|\omega|} = \iint dr_1 dr_2 \Psi_i^*(r_1)\Psi_j^*(r_2)\frac{\sin|\omega|r_{12}}{r_{12}}(1-\alpha_1\alpha_2)\Psi_k^*(r_2)\Psi_l^*(r_1) \qquad (3.35)$$

The separated terms of the sum in (3.34) represent the contributions of different channels and a probability of the dipole transition is:

$$\Gamma_{\alpha n} = \frac{1}{4\pi}V_{\alpha n\alpha n}^{|\omega_{\alpha n}|}. \qquad (3.36)$$

The corresponding oscillator strength: $gf=\lambda^2\Gamma_{\alpha n}/6.67\cdot10^{15}$, where g is the degeneracy degree, λ is a wavelength in angstroms (3.Å). When calculating the matrix elements in (3.13) one should use the angle symmetry and write the expansion for potentials $\sin|\omega|r_{12}/r_{12}$ in spherical functions as follows [119,120]:

$$\frac{\sin|\omega|r_{12}}{r_{12}} = \frac{\pi}{2\sqrt{r_1 r_2}}\sum_{\lambda=0}^{\infty}(\lambda)J_{\lambda+1/2}(|\omega|r_1)J_{\lambda+1/2}(|\omega|r_2)\hat{P}_\lambda(\cos\boldsymbol{r}_1\boldsymbol{r}_2) \qquad (3.37)$$

where J is the Bessel function of first kind and (3.λ)= 2λ + 1. This expansion is corresponding to usual multipole one for probability of radiative decay. Substitution of the expansion (3.37) to matrix element of interaction gives as follows:

$$V^{\omega}_{1234} = [(j_1)(j_2)(j_3)(j_4)]^{1/2} \sum_{\lambda\mu} (-1)^{\mu} \begin{pmatrix} j_1 j_3 & \lambda \\ m_1 - m_3 & \mu \end{pmatrix} \times \mathrm{Im}[Q^{\mathrm{Qul}}_{\lambda}(1243) + Q^{\mathrm{Br}}_{\lambda}(1243)] \tag{3.38}$$

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. Their detailed definitions are presented in Refs. [119-127,134].

3.5. Results and Conclusions

Here we present the results of computing the energies (3.wavelengths) and oscillator strengths for some transitions in spectra of the Li-like ions (3.Z=21-30). There are considered radiative transitions from ground state to the low-excited states $2s_{1/2} - np_{1/2,3/2}$, $np_{1/2,3/2}$-$nd_{3/2,5/2}$. In table 1 we list our computational results on the wavelengths and oscillator strengths gf (3.upper number in the line "Our work": data, obtained without using the optimized basis set and accounting for the exchange-polarization corrections; lower number in the line "Our work" – with using the optimized basis set and accounting for the exchange-polarization corrections) for $1s^2 2s$ ($3.^2S_{1/2}$) → $1s^2 3p$ ($3.^2P_{1/2}$) transitions in the Li-like ions with Z=21-30.

In Table 1 the data on the wavelengths, oscillator strengths, calculated by Banglin Deng et al [52] (3.in the framework of the relativistic configuration-interaction formalism using multiconfiguration DF wave functions and considering the Breit interaction, QED and nuclear mass corrections), Zhang et al (3.the Dirac-Fock-Slater method and disturbed wave approximation), Martin et al (3.the relativistic quantum defect method),Nahar (3.ab initio calculations including relativistic effects employing the Breit-Pauli R-matrix method) and the NIST data [52-55,153-156] are listed too.

Table 1. The calculated wavelengths, oscillator strengths for $1s^2 2s\ (3.^2S_{1/2}) \rightarrow 1s^2 3p\ (3.^2P_{1/2})$ transitions in the Li-like ions with Z=21-30; V/L is the ratios of the velocity and length gauges values by Banglin Deng et al [52]; Ninv (3.in %) is the gauge non-invariant contribution (3.this work);

Z	Ref.	Wavelength (3.A)	Oscillator strength (3.gf, 10^{-1})	V/L; Ninv (3.%)
21	Banglin Deng et al	16.862	1.2392	V/L=0.117
	NIST	16.861	1.2404	
	Zhang et al	16.856	1.250	
	Martin et al	-	1.24	
	This work	16.860	1.2835 1.2401	Ninv=0.10
22	Banglin Deng et al	15.254	1.2484	V/L=0.128
	NIST	15.253	1.2489	
	Zhang et al	15.249	1.259	
	Nahar	15.3	1.281	
	Martin et al		1.24	
	This work	15.252	1.2967 1.2492	Ninv=0.11
24	Banglin Deng et al	12.655	1.2644	V/L=0.149
	NIST	12.665	1.2678	
	Zhang et al	12.647	1.275	
	Nahar	12.7	1.302	
	Martin et al		1.26	
	This work	12.654	1.3140 1.2652	Ninv=0.12
26	Banglin Deng et al	10.664	1.2777	V/L=0.17
	NIST	10.663	-	
	Zhang et al	10.658	1.288	

	Martin et al		1.27	
	This work	10.663	1.3282 1.2796	Ninv=0.12
28	Banglin Deng et al	9.104	1.2889	V/L=0.19
	NIST	9.105	-	
	Zhang et al	9.099	1.299	
	Nahar	9.1	1.339	
	Martin et al		1.28	
	This work	9.103	1.3396 1.2902	Ninv=0.14
30	Banglin Deng et al	7.859	1.2983	V/L=0.21
	Zhang et al	7.854	1.309	
	Martin et al		1.29	
	This work	7.858	1.3492 1.2998	Ninv=0.15

The data by Banglin Deng et al [112] are obtained in the length gauge, and the ratios (3.V/L; in %) of the velocity and length gauges data to check the accuracy of calculations are listed. We also present our values of the gauge non-invariant contribution (3.Ninv; in %). Comparison of the presented data shows that the agreement between the theoretical data and experimental results is more or less satisfactory. One could conclude that the approach presented (3.with using the optimized relativistic PT) can provide sufficiently high accuracy and physically reasonable description of the corresponding wavelengths and oscillator strengths. The fundamental reason for physically reasonable agreement between theory and experiment is connected with the correct taking the exchange-polarization effects into account and using the optimized basis set.

Otherwise, the results, for example, on the oscillator strengths turn out to be worse. It should be noted that an estimate of the gauge-non-invariant contributions (3.the difference between the oscillator strengths values calculated with using the transition operator in the form of “length” and “velocity”) is about 0.15%, i.e., the results for oscillator strengths obtained with using different pho-

ton propagator gauges (3.Coulomb, Babushkin, Landau) are practically equal. This is the evidence of a successful choice of the one-quasiparticle representation. Some difference between the results in Table 1 is also explained by using the different schemes of taking into consideration the correlation and radiative effects.

To conclude, let us underline that the important feature of our approach is using the optimized one-particle representation and accurate accounting for the complex exchange-polarization effects. We believe that the presented consistent approach to construction of the optimal one-quasiparticle representation within the relativistic many-body PT in the theory of multielectron atomic systems can be used with a great efficiency in modern relativistic quantum chemistry, in particular, in calculations of the spectroscopic characteristics of complex molecular systems.

3.6. References

1. Löwdin, Per-Olov. Linear Algebra for quantum theory; Wiley: New York, 1998.
2. Sabin, J.R.; Brändas, E.J. Advances in Quantum Chemistry: Lowdin Volume; Amsterdam: Elsevier, **2017,** 74, 2-392.
3. **Löwdin, Per-Olov. Quantum Theory of Many-Particle Systems. I. Physical Interpretations by means of density matrices, natural spin-orbitals, and convergence problems in the method of configurational interaction. Phys. Rev.** 1955**, 97, 1474.**
4. **Löwdin, Per-Olov; Shull, H**. **Natural Orbitals in the quantum theory of two-electron systems Phys. Rev**. 1956, **101, 1730**
5. **Kobe, D.N. Natural Orbitals, Divergences, and Variational Principles. J. Cjem. Phys.** 1969, **50, 5183.**
6. Davidson E.R., Natural Orbitals. Adv. Quant. Chem. **1972,** 6, 235-266.
7. Suaud N.; Malrieu, J.-P. Natural molecular orbitals: limits of a Lowdin's conjecture, Mol. Phys. 2017, 115(3.21-22), 2684-2695.
8. Maruani, J. The Dirac Electron: From Quantum Chemistry to Holistic Cosmology. Chin. J. Chem.Soc. **2016,** 63,33-48.
9. Lindgren, I. Relativistic many-body theory: A new field-theoretical approach; Springer-Verlag: Berlin, **2011**.

10. Gross, E. K. U.; Dreizler, R. M. Density Functional Theory; Springer: New York, 1995.
11. Bell, K.L.; Berrington, K.A.; Crothers, D.S.F.; Hibbert, A.; Taylor, K.T. Supercomputing, Collision Processes, and Application, Series: Physics of Atoms and Molecules; Springer: New York, **1999**.
12. Kelly, H.P. Correlation Effects in Atoms. Phys. Rev. 1963, 131, 684-692.
13. Kohn, J.W.; Sham, L.J. Self-Consistent Equations Including Exchange and Correlation Effects. Phys. Rev. A **1964,** 140, 1133.
14. Hohenberg, P.; Kohn, W. Inhomogeneous Electron Gas. Phys. Rev. B **1964,** 136, 864.
15. Feller, D.; Davidson, E.R. An approximation to frozen natural orbitals through the use of the Hartree–Fock exchange potential. J. Chem. Phys. **1981,** 74, 3977-3989.
16. Froelich, P.; Davidson, E.R.; Brändas, E. Error estimates for complex eigenvalues of dilated Schrödinger operators. Phys. Rev. A **1983,** 28, 2641.
17. Rittby, M.; Elander, N.; Brändas, E. Scattering in view of the Titchmarsh–Weyl theory. Int. J. Quant. Chem. **1983,** 23, 865-874.
18. Wang, Y.A.; Yung, Y.C.; Chen, Y.K.; Chen, G.H. Communication: Linear-expansion shooting techniques for accelerating self-consistent field convergence. J. Chem. Phys. **2011,** 134, 241103.
19. Thakkar, A.J.; Koga, T.; Tanabe, F.; Teruya, H. Compact Hylleraas-type wave functions for the lithium isoelectronic sequence. Chem. Phys. Lett. **2002**, 366, 95-99.
20. Ho, Y.K. Improved Hylleraas Calculations for Ground State Energies of Lithium Iso-electronic Sequence. Int. J. Quant. Chem. **1981,** XX, 1077-1082.
21. Seaton, M.J. Quantum defect theory. Rep. Prog. Phys. **1983**. 46. 167-258.
22. Martin, I.; Karwowski, J. Quantum defect orbitals and the Dirac second-order equation. J. Phys. B: At. Mol. Opt. Phys. **1991**, 24, 1539-1544.
23. Dyall, K.G.; Faegri Jr., K. Introduction to relativistic quantum theory; Oxford Acad.Oxford, **2007**.
24. Grant, I.P. Relativistic Quantum Theory of Atoms and Molecules. Theory and Computation (3.Series on Atomic, Optical, and Plasma Physics). Springer: New York, **2007**.

25. Sobel'man, I.I. Introduction to theory of atomic spectra. Nauka: Moscow, 1977.
26. Khetselius, O.Yu. Hyperfine structure of atomic spectra; Astroprint: Odessa, **2008**.
27. Glushkov, A.V. Relativistic Quantum theory. Quantum mechanics of atomic systems. Astroprint: Odessa; **2008**.
28. Kiselus, R.S.; Kuplyauskane, A.V.; Rudzikas, Z.B. Theoretical spectra of emission of multicharged ions in plasmas. In Spectroscopy of multicharged ions; Safronova, U.I., Ed.; Nauka: Moscow, **1991**, pp 52-75.
29. Weiss, A.W. Hartree-Fock line strengths for lithium, sodium and copper isoelectronic sequences. J. Quant. Spectr. Rad. Transfer. **1977**, 18(3.5), 481-490.
30. Biemont, E. Theoretical oscillator strengths in the lithium isoelectronic sequence ($3.3 < Z < 22$). Astr. Astrophys. Suppl. Ser. **1977**, 27, 489-493.
31. Lindgard, A.; Nielsen, S.E. Transition probabilities for the alkali isoelectronic sequences: LiI, NaI, KI, RbI, CsI, FrI. Atom.Data.Nucl.Data.Tabl. **1977**, 19, 533-633.
32. Gounand, F. Calculation of radial matrix elements and radiative lifetimes for highly excites states of alkali atoms using the Coulomb approximation. Journ. de Phys. **1979**, 40, 457-460.
33. Das, M.P.; Ramana, M.V.; Rajagopal, A.K. Self-consistent relativistic density-functional theory: Application to neutral U atom and some ions of Li isoelectronic sequence. Phys.Rev.A. **1980**, 22, 9-13.
34. Roy, A.K.; Singh, R.; Deb, B.M. Density functional calculations on triply excited states of lithium isoelectronic sequence. Int.J. Quant. Chem. **199**7, 65, 317-332.
35. Zilitis, V.A. Theoretical determination of the oscillator strengths for the main series of lithium-like ions. Opt. Spectr. **1983**, 55, 215-218
36. Vainstein, L.A.; Safronova, U.I. Energy levels of the He-like and Li-like ions (3.states 1snl, $1s^2$nl with n=2-5). Phys. Scripta. **1985**, 31, 519-532.
37. Johnson, W.R.; Blundell, S.A.; Sapirstein, J. Many-body perturbation-theory calculations of energy levels along the lithium isoelectronic sequence. Phys. Rev. A. **1988** , 37(3.8), 2764-2777.
38. Bylicki, M. Doubly excited Pe and Do Feshbach resonances in the lithium

isoelectronic sequence. Phys. Rev. A. **1993**, 48, 258-263.
39. Yan, Z.C. ; Tambasco, M.; Drake, G.W.F. Energies and oscillator strengths for lithiumlike ions, Phys. Rev. A. 1998, 57, 1652-1662.
40. Schweizer, W.; Faßbinder, P.; Gonzalez-Ferez, R. Model potentials for alkali metal atoms and Li-like ions. Atom. Data. Nucl. Data. Tabl. **1999**, 72**,** 33-55.
41. Godefroid, M.; Froese Fischer, C.; Jonsson, P. Non-relativistic variational calculations of atomic properties in Li-like ions: Li I to O VI. J. Phys. B: Atom. Mol. Opt. Phys. **2001,** 34, 1079-1086.
42. Svinarenko, A.A. Study of spectra for lanthanides atoms with relativistic many- body perturbation theory: Rydberg resonances. J. Phys.: Conf. Ser. **2014,** 548, 012039.
43. Svinarenko, A.A.; Ignatenko, A.V.; Ternovsky, V.B.; Nikola, L.V.; Seredenko, S.S.; Tkach, T.B. Advanced relativistic model potential approach to calculation of radiation transition parameters in spectra of multicharged ions. J. Phys.: Conf. Ser. **2014,** 548, 012047.
44. Zhi-Wen, W.; Ye, Li. Calculations of the transition energies and oscillator strengths for Cu^{26+} ion. J. Atom. Mol. Sci. **2010**, 1, 62-67.
45. Lianhua, Qu; Zhiwen, Wang; Baiwen, Li. Theory of oscillator strength of the lithium isoelectronic sequence. J. Phys. B: At. Mol. Opt. Phys. **1998**, 31, 3601-3608.
46. Zong-Chao, Yan; Drake, G. Theoretical lithium 22S→22P and 22P→32D oscillator strengths. Phys. Rev. A. **1995**, 52, R4316–R4319.
47. Guan, X.-X.; Wang, Z.-W. The hyperfine structure of the 1s2ns2S and 1s2np2P states (3.n = 2; 3; 4; and 5) for the lithium isoelectronic sequence. Eur. Phys. J. D. **1998**, 2, 21-27.
48. Chen, Chao; Wang, Zhi-Wen. Oscillator Strengths for 2s2–2p2P transitions of the lithium isoelectronic sequence from NaIX to CaXVIII. Comm. Theor. Phys. **2005**, 43, 305-308.
49. Guan, Xiaoxu; Li, Baiwen. Energies and oscillator strengths of lithium in a strong magnetic field. Phys. Rev. A. **2001**, 63, 043413.
50. Wu Xiao-Li, Yu Kai-Zhi, Gou Bing-Cong, Zhang Meng. Calculations on the hyperfine constants of the ground states for lithium-like system. China Phys. 2007, 16(3.8), 2389-2393.

51. Hu, M-H; Wang, Z-W. Oscillator strengths for 22S–n2P transitions of Li isoelectronic sequence from Z=11-20. Chin. Phys. B. **2009**, 18, 2244-2254.
52. Banglin, Deng.; Gang, Jiang; Chuanyu Zhang. Relativistic configuration-interaction calculations of electric dipole n = 2 − n = 3 transitions for medium-charge Li-like ions. Atom. Dat. and Nucl. Dat. Tabl. **2014,** 100, 1337-1355.
53. Zhang, H.L.; Sampson, D.H.; Fontes, C.J. Relativistic distorted-wave collision strengths and oscillator strengths for the 85 Li-like ions with 8 <Z< 92. Atom. Dat. Nucl. Dat. Tabl. **1990**, 44, 31-77.
54. Nahar, S. N. Relativistic fine structure oscillator strengths for Li-like ions: C IV - Si XII,SXIV,ArXVI,CaXVIII,Ti XX,Cr XXII, Ni XXVI. Astr. and Astrophys. **2002**. 389, 716-728.
55. Martin, I.; Karwowski, J.; Diercksen, G. H. F.; Barrientos, C. Transition probabilities in the lithium sequence. Astr. and Astrophys. Suppl. **1993**, 100(3.3), 595-605.
56. Refaie, A. I. Fine Structure Calculations of Atomic Data for Ar XVI. Journ. Mod. Phys. **2015**, 6, 1609-1630
57. Natarajan,L.; Natarajan, A.; Kadrekar, R. Relativistic fine-structure oscillator strengths for Li-like ions. Phys. Rev. A. **2010**, 82, 062515.
58. Sakho, I. Screening constant by unit nuclear charge calculations of energies and fine structure splitting for Li-Like Ions. Chin. J. Phys. **2014**, 52,
59. Safronova, U.I.; Safronova, M.S. Relativistic many-body calculation of energies, lifetimes, polarizabilities, and hyperpolarizabilities in Li-like Be^{+}. Phys. Rev. A. **2013**, 87, 032502.
60. Glushkov, A.V. Oscillator strengths of Cs and Rb-like ions. Journ. of Applied Spectroscopy. **1992**, 56(3.1), 5-9.
61. Malinovskaya, S.V.; Glushkov, A.V. Calculation of the spectra of potassium-like multicharged ions. Russian Phys. Journal. **1992,** 35(3.11), 999-1004.
62. Buyadzhi, V.V.; Zaichko, P.A.; Gurskaya, M.Y.; Kuznetsova, A.A.; Ponomarenko E.L.; Ternovsky, V.B.; Relativistic theory of excitation and ionization of Rydberg atomic systems in a Black-body radiation field, J. Phys.: Conf. Ser. **2017,** 810, 012047
63. Buyadzhi, V.V.; Zaichko, P.A.; Antoshkina, O.A.; Kulakli, T.A.; Prepelitsa, G.P.; Ternovsky V.B.; Mansarliysky, V.F. Computing of radiation parame-

ters for atoms and multicharged ions within relativistic energy approach: Advanced Code. J. Phys.: Conf. Ser. **2017,** 905, 012003.

64. Glushkov, A.V.; Efimov, V.A.; Gopchenko, E.D.; Dan'kov, S.V.; Polishchyuk, V.N.; Goloshchak, O.P. Calculation of spectroscopic characteristics 4 of alkali-metal dimers on the basis of a model perturbation theory. Optics and Spectr. **1998,** 84(3.5), 670-678.
65. Glushkov, A.V.; Malinovskaya, S.V.; Loboda, A.V.; Shpinareva, I.M.; Prepelitsa, G.P. Consistent quantum approach to new laser-electron-nuclear effects in diatomic molecules. J.Phys.: Conf. Ser. **2006,** 35, 420-424.
66. Glushkov, A.V. Operator Perturbation Theory for Atomic Systems in a Strong DC Electric Field. In Advances in Quantum Methods and Applications in Chemistry, Physics, and Biology, Series: Progress in Theoretical Chemistry and Physics; Hotokka, M., Brändas, E., Maruani, J., Delgado-Barrio, G., Eds.; Springer: Cham, **2013**; Vol. 27, pp 161–177.
67. Glushkov, A.V.; Ambrosov, S.V.; Ignatenko, A.V.; Korchevsky, D.A. DC strong field stark effect for nonhydrogenic atoms: Consistent quantum mechanical approach. Int. Journ. Quant. Chem. **2004,** 99, 936-939.
68. Glushkov, A.V. QED theory of radiation emission and absorption lines for atoms and ions in a strong laser field. AIP Conf. Proc. **2008,** 1058, 134-136.
69. Glushkov, A.V.; Loboda, A.V. Calculation of the characteristics of radiative multiphoton absorption and emission lines when an atom interacts with pulsed laser radiation. J. Appl.Spectr.(3.Springer). **2007,** 74, 305-309.
70. Glushkov, A.V.; Malinovskaya, S.V.; Filatov, V.V. S-Matrix formalism calculation of atomic transition probabilities with inclusion of polarization effects. Sov. Phys. Journal. **1989,** 32(3.12), 1010-1014.
71. Dietz, K.; Heβ, B.A. Single particle orbitals for configuration interaction derived from quantum electrodynamics. Phys. Scripta. **1989,** 39, 682-688.
72. Glushkov, A.V. Relativistic multiconfiguration time-dependent self-consistent-field theory for molecules. Sov. Phys. Journal. **1991**, 34(3.10), 871-876.
73. Glushkov, A.V.; Efimov, V.A.; Gopchenko, E.D.; Dan'kov, S.V.; Polishchyuk, V.N.; Goloshchak, O.P. Calculation of spectroscopic characteristics of alkali-metal dimers on the basis of a model perturbation theory. Optika i Spektr. **1998,** 84(3.5), 747.

74. Glushkov, A.V.; Malinovskii, A.V.; Efimov, V.A.; Kivganov, A.F.; Khokhlov, V.N.; Vitavetskaya, L.A.; Borovskaya, G.A. Calculation of alkaline metal dimers in terms of model perturbation theory. J. Struct. Chem. **1988,** 39(3.2), 179-185.
75. Glushkov, A.V.; Kondratenko, P.A.; Buyadgi V.V.; Kvasikova, A.S.; Sakun, T.N.; Shakhman, A.S. Spectroscopy of cooperative laser electron-γ-nuclear processes in polyatomic molecules. J. Phys.: Conf. Ser. **2014**, 548, 012025.
76. Glushkov, A.V.; Kondratenko, P.A.; Lepikh, Y.I.; Fedchuk, A.P.; Lovett, L.; Svinarenko, A.A. Electrodynamical and quantum-chemical approaches to modeling the electrochemical and catalytic processes on metals, metal alloys, and semiconductors. Int. Journ. Quant. Chem. **2009,** 109(3.14), 3473-3481.
77. The Fundamentals of Electron Density, Density Matrix and Density Functional Theory in Atoms, Molecules and the Solid State, Series: Progress in Theoretical Chemistry and Physics. Gidopoulos, N. and Wilson, S., Eds.; Springer: Dordrecht, **2004**.
78. Malinovskaya, S.V.; Dubrovskaya, Yu.V.; Vitavetskaya, L.A. Advanced quantum mechanical calculation of the beta decay probabilities. AIP Conf. Proc. **2005**, 796, 201-205.
79. Filatov, M.; Cremer, D. A gauge-independent zeroth-order regular approximation to the exact relativistic Hamiltonian—Formulation and applications. J. Chem. Phys. **2005**, 122, 044104.
80. Zeng, T.; Fedorov, D.G.; Schnidt, M.W.; Klobukowski M. Two-component natural spinors from two-step spin-orbit coupled wave functions. J. Chem. Phys. **2011,** 134, 214107.
81. Hakel P., Mancini R., Abdalah J. etal. X-ray line polarization spectroscopy of Li-like Si satellite spectra. J. Phys. B: At. Mol. Phys. **2009**, 42, 085701.
82. Beiersdorfer, P.; Trabert, E.; Brown, G.V.; Clementson, J.; Thorn, D.B.; Chen, M.H.; Cheng, K.T. Hyperfine Splitting of the 2s1/2 and 2p1/2 Levels in Li- and Be-like Ions of 141Pr. Phys. Rev. Lett**. 2014**, 112, 233003
83. Ivanova, E.P. Highly efficient tabletop x-ray laser at λ=41.8 nm in Pd-like xenon pumped by optical-field ionization in a cluster jet. Phys. Rev. A. **2011,** 84, 043829.
84. Ivanova, E.P.; Grant, I.P. Oscillator strength anomalies in the neon isoelectronic sequence with applications to x-ray laser modeling. J. Phys.B: At.

Mol. Opt. Phys. **1998,** 31, 2871-2880.

85. Le Bigot, E.O.; Boucard, S.; Covita, D.S.; Gotta, D.; Gruber, A.; Hirtl, A.; Fuhrmann, H.; Indelicato, P.; dos Santos, J.M.F.; Schlesser, S.; Simons, L.M.; Stingelin, L.; Trassinelli, M.; Veloso, J.F.; Wasser, A.; Zmeskal J. High-precision x-ray spectroscopy in few-electron ions. Phys. Scripta. **2009**, T134, 014015.
86. Indelicato, P.; S. Covita, D.S.; Gotta, D.; Gruber, A.; Hirtl, A.; Fuhrmann, H.; Le Bigot, E.O.; Schlesser, S.; dos Santos, J.M.F.; Simons, L.M.; Stingelin, L.; Trassinelli, M.; Veloso, J.F.; Wasser, A.; Zmeskal J. Highly charged ion X-rays from Electron–Cyclotron Resonance Ion Sources. Nucl. Instr. Meth. in Phys. Res. A. **2007**, 580, 8-13.
87. Koshelev, K.V.; Labzowsky, L.N.; Tupitsyn, I.I. The interelectron interaction corrections to the hyperfine structure of the $2p_{3/2}$ state in Li-like, B-like and N-like Bi ions. J. Phys. B: At. Mol. Opt. Phys. **2004**, 37, 843-851.
88. Pavlov, R.; Mihailov, L.; Velchev, Ch.; Dimitrova-Ivanovich, M.; Stoyanov, Zh.; Chamel, N.; Maruani, J. Effects induced by nuclear deformations and electron correlations on the ground-state energy of low and multiply charged helium like ions in high-temperature plasmas. J.Phys.: Conf. Ser. **2010,** 253, 012075
89. Glushkov, A.V.; Malinovskaya, S.V.; Chernyakova Y.G.; Svinarenko, A.A. Cooperative laser-electron-nuclear processes: QED calculation of electron satellites spectra for multi-charged ion in laser field. Int. Journ. Quant. Chem. **2004,** 99, 889-893.
90. Glushkov, A.V.; Malinovskaya, S.V.; Prepelitsa, G.P.; Ignatenko, V.M. Manifestation of the new laser-electron nuclear spectral effects in the thermalized plasma: QED theory of co-operative laser-electron-nuclear processes. J. Phys.: Conf. Ser. **2005,** 11, 199-206.
91. Glushkov, A.V.; Malinovskaya, S.V.; Loboda, A.V.; Shpinareva, I.M.; Gurnitskaya, E.P.; Korchevsky, D.A. Diagnostics of the collisionally pumped plasma and search of the optimal plasma parameters of x-ray lasing: calculation of electron-collision strengths and rate coefficients for Ne-like plasma. J. Phys.: Conf. Ser. **2005,** 11, 188-198.
92. Glushkov, A.V.; Ambrosov, S.V.; Loboda, A.V.; Gurnitskaya, E.P.; Prepelitsa, G.P. Consistent QED approach to calculation of electron-collision

excitation cross sections and strengths: Ne-like ions. Int. J. Quantum Chem. **2005,** 104, 562-569.

93. Glushkov, A.V.; Loboda, A.V.; Gurnitskaya, E.P.; Svinarenko, A.A. QED theory of radiation emission and absorption lines for atoms in a strong laser field. Phys. Scripta. **2009,** T135, 014022.
94. Florko, T.A.; Tkach, T.B.; Ambrosov, S.V.; Svinarenko, A.A. Collisional shift of the heavy atoms hyperfine lines in an atmosphere of the inert gas. J. Phys.: Conf. Ser. **2012**, 397, 012037.
95. Buyadzhi, V.V. Laser multiphoton spectroscopy of atom embedded in Debye plasmas: multiphoton resonances and transitions. Photoelectronics. **2015,** 24, 128-133.
96. Buyadzhi, V.V.; Chernyakova, Yu.G.; Smirnov, A.V.; Tkach, T.B. Electron-collisional spectroscopy of atoms and ions in plasma: Be-like ions. Photoelectronics. **2016,** 25, 97-101.
97. Buyadzhi, V.V.; Chernyakova, Yu.G.; Antoshkina, O.A.; Tkach, T.B. Spectroscopy of multicharged ions in plasmas: Oscillator strengths of Be-like ion Fe. Photoelectronics. **2017,** 26, 94-102.
98. Khetselius, O.Yu. Relativistic Energy Approach to Cooperative Electron-γ-Nuclear Processes: NEET Effect In Quantum Systems in Chemistry and Physics, Series: Progress in Theoretical Chemistry and Physics; Nishikawa, K., Maruani, J., Brändas, E., Delgado-Barrio, G., Piecuch, P., Eds.; Springer: Dordrecht, **2012;** Vol. 26, pp 217-229.
99. Khetselius, O.Yu. Relativistic perturbation theory calculation of the hyperfine structure parameters for some heavy-element isotopes. Int. Journ.Quant.Chem. **2009,** 109, 3330-3335.
100. Khetselius, O.Yu. Relativistic calculation of the hyperfine structure parameters for heavy elements and laser detection of the heavy isotopes. Phys.Scripta. **2009,** 135, 014023.
101. Khetselius, O.Yu. Optimized Perturbation Theory for Calculating the Hyperfine Line Shift and Broadening of Heavy Atoms in a Buffer Gas. In Frontiers in Quantum Methods and Applications in Chemistry and Physics, Series: Progress in Theoretical Chemistry and Physics; Nascimento, M., Maruani, J., Brändas, E., Delgado-Barrio, G., Eds.; Springer: Cham, **2015;** Vol. 29, pp. 55-76.

102. Khetselius, O.Yu. Quantum structure of electroweak interaction in heavy finite Fermi-systems. Astroprint: Odessa, **2011**.
103. Serot, B.D.; Walecka, J.D. Advances in Nuclear Physics: The Relativistic Nuclear Many Body Problem. Plenum Press; New York, **1986**.
104. Tomaselli, M.; Schneider, S.M.; Kankeleit, E.; Kuhl, T. Ground-state magnetization of ^{209} Bi in a dynamic-correlation model. Phys. Rev. C **1995,** 51, 2989.
105. Nagasawa, T.; Naga, A.; Nakano, M. Hyperfine splitting of hydrogen like atoms based on relativistic mean field theory, Phys. Rev. C **2004,** 69, 034322.
106. Glushkov, A.V.; Rusov, V.D.; Ambrosov, S.V.; Loboda, A.V. Resonance states of compound super-heavy nucleus and EPPP in heavy nucleus collisions In New Projects and New Lines of Research in Nuclear Physics. Fazio, G., Hanappe, F., Eds.; World Scientific: Singapore, **2003**, 126-132.
107. Glushkov, A.V. Spectroscopy of atom and nucleus in a strong laser field: Stark effect and multiphoton resonances. J. Phys.: Conf. Ser. **2014**, 548, 012020
108. Shahbaz, A.; Muller, C.; Staudt, A.; Burvenich, T.J.; Keitel, C.H. Nuclear Signatures in High-Order Harmonic Generation from Laser-Driven Muonic Atoms. Phys. Rev. Lett. **2007,** 98, 263901.
109. Mohr, P.J. Phys. Self-energy of the n = 2 states in a strong Coulomb field. Phys. Rev. A **1982,** 26, 2338.
110. Indelicato, P. Relativistic effects in few-electron heavy atoms. Ab initio evaluation of levels energy and transition probabilities. Phys. Scripta. **1996**, T65, 57-62.
111. Blundell, S.A.; Sapirstein, J.; Johnson, W.R. High-accuracy calculation of parity nonconservation in cesium and implications for particle physics. Phys. Rev. D. **1992**, 45, 1602-1612.
112. Johnson, W.R.; Sapirstein, J.; Blundell, S.A. Atomic structure calculations associated with PNC experiments in atomic cesium. Phys. Scripta **1993,** 46, 184.
113. Persson, H.; Lindgren, I.; Salomonson, S.; Lindgren, I. Two-electron Lamb-shift calculations on heliumlike ions. Phys. Rev. Lett. **1996,** 76, 204–207.

114. Flambaum, V.V.; Ginges, J.S.M. Radiative potential and calculations of QED radiative corrections to energy levels and electromagnetic amplitudes in many-electron atoms. Phys. Rev. A **2005,** 72, 052115.
115. Yerokhin, V.; Artemyev, A.; Shabaev, V.M. QED treatment of electron correlation in Li-like ions. Phys. Rev. A. **2007**, 75, 062501.
116. Bieron, J.; Pyykkő, P.; Jonsson, P. Nuclear quadrupole moment of ^{201}Hg. Phys. Rev. A. **2005,** 71, 012502.
117. Glushkov, A.V.; Gurnitskaya, E.P.; Loboda, A.V. Advanced Quantum Mechanical Calculation of Superheavy Ions: Energy Levels, Radiation and Finite Nuclear Size Effects. AIP Conference Proceedings. **2005,** 796, 217-220.
118. Derevianko, A.; Porsev, S.G. "Dressing" lines and vertices in calculations of matrix elements with the coupled-cluster method and determination of Cs atomic properties. Phys. Rev. A. **2005**, 71, 032509.
119. Ivanov, L.N.; Ivanova, E.P. Atomic ion energies for Na-like ions by a model potential method Z = 25–80. Atom. Data Nucl. Data Tabl. **1979,** 24, 95-109.
120. Driker, M.N.; Ivanova, E.P.; Ivanov, L.N.; Shestakov, A.F. Relativistic calculation of spectra of 2-2 transitions in O-and F-like atomic ions. J.Quant.Spectr. Rad. Transfer. **1982,** 28, 531-535.
121. Ivanov, L.N.; Ivanova, E.P.; Aglitsky, E.V. Modern trends in the spectroscopy of multicharged ions. Phys. Rep. **1988,** 166, 315-390.
122. Ivanova, E.P.; Ivanov, L.N.; Glushkov, A.V.; Kramida, A.E. High order corrections in the relativistic perturbation theory with the model zeroth approximation, Mg-Like and Ne-Like Ions. Phys. Scripta 1985, 32, 513-522.
123. Ivanova, E.P.; Gulov, A.V. Theoretical investigation of the neon isoelectronic sequence. Atom. Data Nuc. Data Tabl. **1991,** 49, 1-64.
124. Ivanov, L.N.; Ivanova, E.P. Method of Sturm orbitals in calculation of physical characteristics of radiation from atoms and ions. JETP. **1996,** 83, 258-266.
125. Ivanov, L.N.; Ivanova, E.P.; Knight, L. Energy approach to consistent QED theory for calculation of electron-collision strengths: Ne-like ions. Phys. Rev. A. **1993,** 48, 4365-4374.
126. Glushkov, A.V.; Ivanov, L.N.; Ivanova, E.P. Autoionization Phenomena

in Atoms. Moscow University Press, Moscow, **1986,** 58-160

127. Glushkov, A.V.; Ivanov, L.N. Radiation decay of atomic states: atomic residue polarization and gauge noninvariant contributions. Phys. Lett. A **1992,** 170, 33-36.

128. Glushkov A.V.; Ivanov, L.N. DC strong-field Stark effect: consistent quantum-mechanical approach. J. Phys. B: At. Mol. Opt. Phys. **1993,** 26, L379-386.

129. Glushkov, A.V. Relativistic and Correlation Effects in Spectra of Atomic Systems. Astroprint: Odessa, **2006**.

130. Glushkov, A.V. Relativistic polarization potential of a many-electron atom. Sov. Phys. Journal. **1990**, 33(3.1), 1-4.

131. Glushkov, A.V. Negative ions of inert gases. JETP Lett. **1992,** 55, 97-100.

132. Glushkov, A.V. Energy approach to resonance states of compound superheavy nucleus and EPPP in heavy nuclei collisions In Low Energy Antiproton Physics; Grzonka, D., Czyzykiewicz, R., Oelert,W., Rozek, T., Winter, P., Eds.; AIP: New York, AIP Conf. Proc. **2005**, 796, 206-210.

133. Glushkov, A.V. Spectroscopy of cooperative muon-gamma-nuclear processes: Energy and spectral parameters J. Phys.: Conf. Ser. **2012,** 397, 012011

134. Glushkov, A.V. Advanced Relativistic Energy Approach to Radiative Decay Processes in Multielectron Atoms and Multicharged Ions. In Quantum Systems in Chemistry and Physics: Progress in Methods and Applications, Series: Progress in Theoretical Chemistry and Physics; Nishikawa, K., Maruani, J., Brandas, E., Delgado-Barrio, G., Piecuch, P., Eds.; Springer: Dordrecht, **2012**; Vol. 26, pp 231–252.

135. Glushkov, A.V.; Butenko, Yu.V.; Serbov, N.G.; Ambrosov, S.V.; Orlova, V.E.; Orlov, S.V.; Balan, A.K.; Dormostuchenko, G.M. Calculation of the oscillator strengths in Fr-like multiply charged ions. Journ. of Applied Spectrosc. **1996,** 63(3.1), 28-30.

136. Glushkov, A.V.; Butenko, Yu.V.; Serbov, N.G.; Ambrosov, S.V.; Orlova, V.E.; Orlov, S.V.; Balan, A.K.; Dormostuchenko, G.M. Calculation and extrapolation of oscillator strengths in Rb-like, multiply charged ions. Russian Phys. Journ. **1996**, 39(3.1), 81-83.

137. Glushkov, A.V. Correction for exchange and correlation effects in mul-

tielectron system theory. Journ. of Struct. Chem. **1990**, 31(3.4), 529-532.
138. Khetselius, O.Yu. Relativistic Hyperfine Structure Spectral Lines and Atomic Parity Non-conservation Effect in Heavy Atomic Systems within QED Theory. AIP Conf. Proceedings. **2010,** 1290(3.1), 29-33.
139. Khetselius, O.Yu. Relativistic Calculating the Spectral Lines Hyperfine Structure Parameters for Heavy Ions. AIP Conf. Proc. **2008,** 1058, 363-365.
140. Khetselius, O.Yu. Hyperfine structure of energy levels for isotopes ^{73}Ge, ^{75}As, ^{201}Hg. Photoelectronics. **2007,** 16, 129-132.
141. Khetselius, O.Yu.; Gurnitskaya, E.P. Sensing the electric and magnetic moments of a nucleus in the N-like ion of Bi. Sensor Electr. and Microsyst. Techn. **2006,** 3, 35-39.
142. Khetselius O.Yu.; Gurnitskaya, E.P. Sensing the hyperfine structure and nuclear quadrupole moment for radium. Sensor Electr. and Microsyst. Techn. **2006,** 2, 25-29.
143. Khetselius, O.Yu. Atomic parity non-conservation effect in heavy atoms and observing P and PT violation using NMR shift in a laser beam: To precise theory. J. Phys.: Conf. Ser. **2009,** 194, 022009
144. Ivanov, L.N.; Letokhov, V.S. Doubly excited autoionization states of multielectron atoms. Com. Mod. Phys. D: At. Mol. Phys. **1985,** 4, 169–184.
145. Ignatenko, A.V. Probabilities of the radiative transitions between Stark sublevels in spectrum of atom in an DC electric field: New approach. Photoelectronics, **2007,** 16, 71-74.
146. Glushkov, A.V.; Ambrosov, S.V.; Ignatenko, A.V. Non-hydrogenic atoms and Wannier-Mott excitons in a DC electric field: Photoionization, Stark effect, Resonances in ionization continuum and stochasticity. Photoelectronics, **2001,** 10, 103-106.
147. Glushkov, A.V.; Gurskaya, M.Yu.; Ignatenko, A.V.; Smirnov, A.V.; Serga, I.N.; Svinarenko, A.A.; Ternovsky, E.V. Computational code in atomic and nuclear quantum optics: Advanced computing multiphoton resonance parameters for atoms in a strong laser field. J. Phys.: Conf. Ser. **2017**, 905, 012004.
148. Glushkov, A.V. True effective molecular valency hamiltonian in a logical semiempricial theory. Journal of Structural Chem. **1988**, 29(3.4), 495-501
149. Glushkov, A.V. Polarization effects in ethylene molecule spectrum calcu-

lation. Journal of Appl. Spectroscopy. **1992,** 56 (3.3), 309–312.

150. Glushkov, A.V. New form of effective potential to calculate polarization effects of the π-electronic states of organic molecules, J. Struct. Chem. **1994**, 34, 659–665.

151. Glushkov, A.V.; Antonenko, T.N.; Serbov, N.G.; Ambrosov, S.V.; Orlova, V.E.; Orlov, S.V.; Dormostuchenko, G.M.; Chernyshova, A.K. Transition energies and oscillator strengths in the spectrum of a CO molecule. Journ. of Applied Spectrosc. **1996,** 63 (3.2), 279-282.

152. Glushkov, A.V.; Serbov, N.G.; Ambrosov, S.V.; Orlova, V.E.; Dormostuchenko, G.M.; Troitskaya, O.V. Effective account of 2 p-2 h excitations in molecular calculations by the equation-of-motion method. Journ. of Structural Chem. **1995,** 36(3.4), 557-564.

153. Martin, G.A.; Wiese, W.L. Atomic oscillator-strength distributions in spectral series of Li isoelectronic sequence. Phys. Rev. A. **1976**, 13**,** 699-714.

154. Martin, G.A.; Wiese, W.L. Tables of critically evaluated oscillator strengths for lithium isoelectronic sequence. J. Phys. Chem. Ref. Data. **1976**, 5, 537-570.

155. Moore, C. NBS Spectra Database; NBS: Washington, **1987**.

156. Martin, G. NIST Spectra Database, version 2.0; NIST: Washington, **2004** (3.http://physics.nist.gov.asd).

CHAPTER 4. ADVANCED QUANTUM APPROACH IN RADIATIVE AND COLLISIONAL SPECTROSCOPY OF MULTICHARGED IONS

4.1 Introduction

In this chapter an advanced relativistic quantum approach to computing the important radiative and collisional characteristics of multicharged ions in the Debye plasmas is presented. The approach is based on the relativistic energy formalism (4.the Gell-Mann and Low formalism) and relativistic many-body perturbation theory (4.PT) with the Dirac-Debye shielding model Hamiltonian for electron-nuclear and electron-electron systems. The optimized one-electron representation in the PT zeroth approximation is constructed by means of the correct treating the gauge dependent multielectron contribution of the lowest PT corrections to the radiation widths of atomic levels. The computational results for the oscillator strengths and energy shifts due to the plasma's environment effect, the effective collision strengths for the Be- and Ne-like ions of Fe, Zn and Kr embedded to different types of plasmas environment (4.with temperature 0.02-2 keV and electron density 10^{16}-10^{24} cm^{-3}) are presented and analyzed.

The properties of laboratory, thermonuclear (4.tokamak), laser-produced, astrophysical plasmas have drawn considerable attention over the last decades [1-5]. It is known that multicharged ions play an important role in the diagnostics of a wide variety of plasmas [1-23].

Electron-ion collisions involving multiply charged ions, as well as various radiation and radiation-collisional processes, predetermine the quantitative characteristics of the energy balance of the plasmas [1-4,13-20]. For this reason, the plasmas modelers and diagnosticians require absolute cross sections for these processes. The cross sections for electron-impact excitation of ions are needed to interpret spectroscopic measurements and for simulations of plasmas using collisional-radiative models. Above other important factors to studying electron-collisional spectroscopy of ions one should mention the known X-ray laser problem.

It has stimulated a great number of papers, devoted to modelling the elementary processes in laser, collisionally pumped plasmas and construction of the first VUV and X-ray lasers with using plasmas of Li-, Ne-like ions as an active

medium. Very useful data on the X-lasers problem are collected in the papers by Ivanova et al (4.see [3,4] and Refs. therein).

Such well-known atomic methods as the multi-configuration Dirac–Fock, R-, T-matrix, relativistic distorted-wave methods, 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 others have been intensively applied to problems considered. At present time a considerable interest has been encapsulated to studying elementary atomic processes in plasmas environments because of the plasmas screening effect on the plasmas-embedded atomic systems. In many papers the calculations of various atomic and ionic systems embedded in the Debye plasmas have been performed [13-20, 29-33]; it is well-known that the Debye model is justified only in the limit of high temperature and low density. However, a development of the advanced computational quantum methods and models for the further accurate computing oscillator strengths, electron-collisional strengths and cross-sections for the atomic ions in plasmas, including the Debye plasmas, remained a very actual and difficult problem (4.for example, see [1-42] and Refs. therein) . To say strictly, solving of the whole problem requires a development of the quantum-electrodynamical approach as the most consistent one to problem of the Coulomb many-body system.

In Refs. [39-42] the fundamentals of an advanced quantum approach to studying spectroscopic characteristics of the multicharged ions in the Debye plasmas, in particular, computing the electron-ion collision strengths, cross-sections etc have been presented. The approach is based on the relativistic energy formalism (4.the Gell-Mann and Low formalism) and relativistic many-body perturbation theory (4.PT) with the Debye shielding model Hamiltonian for electron-nuclear and electron-electron systems. It is worth to underline that our method of the relativistic many-body PT formalism is constructed on the base of the same ideas as the well-known PT approach with the model potential zeroth approximation by Ivanov-Ivanova et al [43-51]. However there are a few fundamental differences. For example, in our case the PT zeroth approximation [39,40] is in fact the Dirac-Debye-Hückel one. The optimized one-electron representation in the PT zeroth approximation is constructed by means of the correct treating the gauge dependent multielectron contribution of the lowest PT

corrections to the radiation widths of atomic levels [51,52]. In order to calculate the radiative and collisional parameters an effective gauge-invariant version of relativistic energy approach is used [51-54].

It is important to note that a model relativistic energy approach in a case of a multielectron atom has been developed by Ivanov-Ivanova *et al* [43-50]. A generalized gauge-invariant version of relativistic energy approach in a case of the multielectron atomic systems has been developed by Glushkov-Ivanov-Ivanova (4.see Refs. [51-56]).

Earlier it has been successfully applied to solve many actual problems of modern atomic, nuclear and even molecular optics and spectroscopy etc (4.see [57-93] and Refs. therein). The computation results on the oscillator strengths and energy shifts due to the plasmas environment effect, the electron-collision strengths, collisional excitation and de-excitation rates for the Be- and Ne-like ions of argon and nickel for the plasmas environment with the temperature 0.02-2 keV and the electron density n_e= 10^{16}-10^{24} cm^{-3} are listed in Refs. [39,41]. In this paper, we briefly describe the key points of our approach, focus on some subtle details not previously described, and present new results on the oscillator strengths, energy shifts, effective collision forces for Be- and Ne-like Fe, Kr, and Zn ions in a plasmas environment with the temperature 0.02-2 keV and n_e=10^{22}-10^{24} cm^{-3}.

4.2 Radiative and collisional spectroscopy of multicharged ions: Relativistic many-body perturbation theory and relativistic energy approach

4.2.1 Relativistic many-body perturbation theory with Dirac-Debye shielding model zeroth approximation

In order to calculate different characteristics such as oscillator strengths and energy shifts due to the plasmas environment effect, the electron-collision strengths, collisional excitation and de-excitation rates etc we use an advanced generalized relativistic energy approach combined with the relativistic many-body PT with the the Dirac- Debye zeroth approximation.

In the theory of 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 [37,43-48]. In constructing M, the Gell-Mann and Low adiabatic formula for ΔE is used. The secular matrix elements are already complex in the PT second order (4.the first order on the inter-electron interaction). The total energy shift of the state is presented in the form:

$$\Delta E = \mathrm{Re}\Delta E + \mathrm{i}\ \mathrm{Im}\Delta E,$$
$$\mathrm{Im}\ \Delta E = -\Gamma/2, \qquad (4.1)$$

where Γ is interpreted as the level width. Their imaginary parts are connected with the radiation decay possibility. It is important to note that the computing the energies and radiative transition matrix elements is reduced to calculation and the further diagonalization of the complex matrix M and determination of matrix of the coefficients with eigen state vectors $B^{IK}_{ie,iv}$ [38, 48-51]. To calculate all necessary matrix elements one must use the basis set of the one-quasiparticle relativistic functions. Numerous calculations of the atomic elementary processes characteristics have shown [13-20, 29-33] that their adequate description requires using the optimized wave functions and an accurate accounting for the exchange-correlation effects.

In Ref. [52] the “ab initio” optimization principle for construction of an effective one-quasiparticle representation has been proposed. The minimization of the gauge dependent multielectron contribution of the lowest QED PT corrections to the radiation widths of atomic levels, determined by the imaginary part of an energy shift ΔE, is used. In the fourth order of QED PT there are diagrams appearing, whose contribution into the $\mathrm{Im}\Delta E$ accounts for the polarization effects. This contribution describes collective effects and it is dependent upon the electromagnetic potentials gauge (4.the gauge non-invariant contribution ΔE_{ninv}). This value is considered to be the typical representative of the electron correlation effects, whose minimization is a reasonable criterion in the searching for the optimal PT one-electron basis. Let us note that this topic has always been of fundamental importance in quantum chemistry throughout its development

(4.see e.g. Refs. [94-130], where some alternative approaches to optimization are presented).

The detailed formulation of the relativistic many-body PT with the Debye shielding model Dirac Hamiltonian for electron-nuclear and electron-electron systems has been earlier presented [39-42]. Here we will focus on the key points. The Dirac-Debye shielding model Hamiltonian for electron-nuclear and electron-electron subsystems can be defined as follows (4.atomic units are used):

$$H = \sum_i [\alpha cp - \beta mc^2 - Z\exp(-\mu r_i)/r_i] + \sum_{i>j} \frac{(1-\alpha_i\alpha_j)}{r_{ij}} \exp(-\mu r_{ij}), \qquad (4.2)$$

where c is the velocity of light and Z is a charge of the atomic ion nucleus, ω_{ij} is the transition frequency; α_i ,α_j are the Dirac matrices. The plasmas environment effect is modelled by the shielding parameter μ , which describes a shape of the long-range potential. The parameter μ is connected with the plasmas parameters such as temperature T and the charge density n as follows:

$$\mu \sim \sqrt{e^2 n / k_B T} \ . \qquad (4.3a)$$

Here e is the electron charge and k_B is the Boltzmann constant. The density n is given as a sum of the electron density N_e and the ion density N_k of the k-th ion species with the nuclear charge q_k :

$$n = N_e + \sum_k q_k^2 N_k \ . \qquad (4.3b)$$

It is worth to note that indeed the Debye screening for the atomic electrons in the Coulomb field of nuclear charge is well understood due to the presence of the surrounding plasma electrons with high mobility. On the other hand, the contribution due to the Debye screening between electrons would be of smaller magnitude orders. Majority of the previous works on the spectroscopy study have considered the screening effect only in the electron-nucleus potential where the electron-electron interaction potential is truncated at its first term of the standard exponential expansion for its dominant contribution [13-18]. However,

as the authors [17,35] note, it is also important to take into account the screening in the electron- electron interactions for large plasma strengths to achieve more realistic results in the search for stability of the atomic structure in the plasma environment.

It is not difficult to make some simple estimates for the shielding parameter. For example, under typical laser plasmas conditions of $T\sim$ 1keV and $n\sim 10^{22}$ cm^{-3} the parameter μ is of the order of 0.1 in atomic units; in the EBIT plasmas $T\sim$ 0.05keV, $n\sim 10^{18}$ cm^{-3} and $\mu\sim 10^{-3}$. We are interested in studying the spectral parameters of ions in plasmas with the temperature $T\sim$ 0.1-1keV (4.10^6-10^7K) and $n\sim 10^{24}$-10^{26} cm^{-3} ($4.\mu\sim 10^{-2}$-10^{-1}).

The formalism of the relativistic many-body PT is further constructed in the same way as the PT formalism in Refs. [43-51]. In the PT zeroth approximation one should use a mean-field potential, which includes the Yukawa-type potential (4.insist of the pure Coulomb one) plus exchange Kohn-Sham potential and additionally the modified Lundqvist-Gunnarsson correlation potential (4.with the optimization parameter *b*) as in Refs. [52,53]. As an alternative one could use an optimized model potential by Ivanova-Ivanov (4.for Ne-like ions) [38,43], which is calibrated by means of the special ab initio procedure within the relativistic energy approach [52].

The most complicated problem of the relativistic PT computing the radiative and collisional characteristics of the multielectron multicharged ions is an accurate, precise accounting for the exchange-correlation effects (4.including polarization and screening effects, a continuum pressure and other ones) as the effects of the PT second and higher orders . Using the standard Feynman diagram technique one should consider different kinds of diagrams, in particular, the polarization and ladder ones, which describe the polarization and screening exchange-correlation effects.

An effective approach to accounting for the polarization diagrams contributions is adding the effective two-quasiparticle polarizable operator into the PT first order matrix elements. In Ref. [47] the corresponding non-relativistic polarization functional has been derived. The generalized relativistic expression has been derived in the Refs. [53,63] and used in our work. According to Ref. [63], the polarization potential (4.“direct” polarization part) is as follows:

$$V_{d-pol}^{Rel}(r_1 r_2) = X \{ \int \frac{d\tilde{r} \left(\rho_c^{(0)}(\tilde{r})\right)^{1/3} \theta(\tilde{r})}{|r_1 - \tilde{r}| \cdot |\tilde{r} - r_2|} -$$

$$- \int \frac{d\tilde{r} \left(\rho_c^{(0)}(\tilde{r})\right)^{1/3} \theta(\tilde{r})}{|r_1 - \tilde{r}|} \int \frac{d\tilde{r} \left(\rho_c^{(0)}(\tilde{r})\right)^{1/3} \theta(\tilde{r})}{|\tilde{r} - r_2|} \Big/ [\int d\tilde{r} \left(\rho_c^{(0)}(\tilde{r})\right)^{1/3} \theta(\tilde{r})]^{1/3} \},$$

$$\theta(r) = \left\{ 1 + \left[3\pi^2 \cdot \rho_c^{(0)}(r) \right]^{2/3} / c^2 \right\}^{1/2}, \qquad (4.4)$$

where X is the numerical coefficient, $\rho_c^{(0)}(r)$ is the ionic core electron density. The corresponding expression for the "exchange" polarization potential is presented in Refs. [53,63].

4.2.2 Relativistic energy approach in radiative and collisional spectroscopy of multicharged ions

The justification of the relativistic energy approach in the scattering problem is in details described in Refs. [38,42,50-54]. Below we concern the most principal points using the results [38,42,50,52]. Further for definiteness, let us consider a collisional de-excitation of, say, the Ne-like ion:

$$(2j_{iv})^{-1} 3j_{ie}[J_i M_i],\ \varepsilon_{in}) \rightarrow (4.\Phi_o, \varepsilon_{sc}). \qquad (4.5)$$

Here Φ_o is the state of the ion with the closed shells (4.ground state of the Ne-like ion); J_i is the total angular moment of the initial target state; indices *iv, ie* are related to the initial states of a vacancy and an electron; indices ε_{in} and ε_{sc} are the incident and scattered energies, respectively to the incident and scattered electrons. The initial state of the system "atom plus free electron" can be written as

$$| I >= a_{in}^{+} \sum_{m_{iv}, m_{ie}} a_{ie}^{+} a_{iv} \Phi_o C_{m_{ie}, m_{iv}}^{J_i, M_i} \qquad (4.6a)$$

where $C_{m_{ie}, m_{iv}}^{J_i, M_i}$ is the Clebsh-Gordan coefficient. The final state is as follows:

$$| F >= a_{sc}^{+}\Phi_o , \qquad (4.6b)$$

where Φ_o is the state of an ion with closed electron shells (4.ground state of Ne-like ion), |*I*> represents three-quasiparticle (4.3QP) state , and |*F*> represents the one-quasiparticle (4.1QP) state.

The scattered part of energy shift Im ΔE appears firstly in the atomic PT second order (4.the fourth order of the QED PT) in the form of integral over the scattered electron energy ε_{sc} [50-52]:

$$\int d\varepsilon_{sc} G(\varepsilon_{iv},\varepsilon_{ie},\varepsilon_{in},\varepsilon_{sc})/(\varepsilon_{sc}-\varepsilon_{iv}-\varepsilon_{ie}-\varepsilon_{in}-i0) \qquad (4.7a)$$

$$\mathrm{Im}\Delta E = \pi\, G(\varepsilon_{iv},\varepsilon_{ie},\varepsilon_{in},\varepsilon_{sc}) . \qquad (4.7b)$$

Here *G* is a definite squired combination of the two-electron matrix elements (4.2). As usually, the value

$$\sigma\text{=-2 Im}\Delta E \qquad (4.8)$$

represents the collisional cross-section if the incident electron eigen-function is normalized by the unit flow condition and the scattered electron eigen-function is normalized by the energy δ function. The collisional de-excitation cross section can further defined as follows:

$$\sigma(IK\to 0) = 2\pi \sum_{j_{in},j_{sc}} (2j_{sc}+1)\{\sum_{j_{ie},j_{iv}} < 0 \mid j_{in}, j_{sc} \mid j_{ie}, j_{iv}, J_i > B_{ie,iv}^{IK}\}^2 \qquad (4.9a)$$

The amplitude like combination in (4.9) has the following form:

$$< 0 \mid j_{in}, j_{sc} \mid j_{ie}, j_{iv}, J_i >= \sqrt{(2j_{ie}+1)(2j_{iv}+1)}(-1)^{j_{ie}+1/2} \times \sum_{\lambda}(-1)^{\lambda+J_i} \times$$
$$\times \{\delta_{\lambda,J_i}/(2J_i+1) Q_\lambda(sc,ie;iv,in) + \begin{bmatrix} j_{in}\cdots j_{sc}\cdots J_i \\ j_{ie}\cdots j_{iv}\cdots\lambda \end{bmatrix} Q_\lambda(ie;in;iv,sc)\} \qquad (4.9b)$$

$$Q_\lambda = Q_\lambda^{\text{Coul-Deb}} + Q_\lambda^{Br} , \qquad (4.9c)$$

where $Q_\lambda^{\text{Coul-Deb}} + Q_\lambda^{Br}$ is the sum of the Coulomb-Debye and Breit matrix elements. The part $Q_\lambda^{\text{Coul-Deb}}$ contains the Slater-like radial R_λ and standard angular S_λ parts as follows (4.for example, see details in Refs. [43,47]):

$$Q_\lambda^{\text{Coul-Deb}} = \{R_\lambda(1243)S_\lambda(1243) + R_\lambda(\tilde{1}24\tilde{3})S_\lambda(\tilde{1}24\tilde{3}) + \\ + R_\lambda(1\tilde{2}4\tilde{3})S_\lambda(1\tilde{2}4\tilde{3}) + R_\lambda(\tilde{1}\tilde{2}4\tilde{3})S_\lambda(\tilde{1}\tilde{2}4\tilde{3})\}. \quad (4.10)$$

Here the tilde designates that the large radial Dirac component f must be replaced by the small Dirac component 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 part is described in details in Refs. [43-47]. In particular, the Breit (4.magnetic) part is usually expressed as follows:

$$Q_\lambda^{Br} = Q_{\lambda,\lambda-1}^{Br} + Q_{\lambda,\lambda}^{Br} + Q_{\lambda,\lambda+1}^{Br} \quad (4.11a)$$

where all terms $Q_{\lambda,\lambda-1}^{Br}, Q_{\lambda,\lambda}^{Br}, Q_{\lambda,\lambda+1}^{Br}$ contains the corresponding radial R_λ and angular S_λ parts, for example:

$$Q_{\lambda,l}^{Br} = \{R_\lambda(12;\tilde{4}\tilde{3})S_\lambda^l(12;\tilde{4}\tilde{3}) + R_\lambda(\tilde{1}\tilde{2};43)S_\lambda^l(\tilde{1}\tilde{2};43) + \\ + R_\lambda(\tilde{1}2;\tilde{4}3)S_\lambda^l(\tilde{1}2;\tilde{4}3) + R_\lambda(\tilde{1}\tilde{2};\tilde{4}\tilde{3})S_\lambda^l(\tilde{1}\tilde{2};\tilde{4}\tilde{3})\}. \quad (4.11b)$$

The detailed expressions for the angular elements are presented in Refs. [39-44].

According to the Eq. (4.1), a probability of the radiative transition is directly connected with imaginary part of electron energy of the system (4.the Ivanov-Ivanov's version of the energy approach [37,38,51]), which can be defined in the lowest order of the PT as follows:

$$\text{Im}\Delta E = -\frac{e^2}{4\pi} \sum_{\substack{\alpha>n>f \\ [\alpha<n\le f]}} V_{\alpha n \alpha n}^{|\omega_{\alpha n}|}, \quad (4.12)$$

where $\sum_{\alpha>n>f}^{-}$ for electron and $\sum_{\alpha<n\le f}^{-}$ for vacancy. The potential V is as follows:

$$V_{ijkl}^{|\omega|} = \iint dr_1 dr_2 \Psi_i^*(r_1)\Psi_j^*(r_2)\frac{\sin|\omega|r_{12}}{r_{12}}(1-\alpha_1\alpha_2)\Psi_k^*(r_2)\Psi_l^*(r_1) \qquad (4.13)$$

The corresponding oscillator strength is defined as:

$$gf = \lambda_g^2 \cdot \Gamma_{\alpha_n} / 6.67 \cdot 10^{15}, \qquad (4.14)$$

where g is the degeneracy degree, λ is a wavelength in angstroms (4.Å).

The total probability of a λ - pole transition is usually represented as a sum of the electric P_λ^E and magnetic P_λ^M parts. The electric (4.or magnetic) λ - pole transition $\alpha \to n$ connects two states with parities which by λ (4. or λ +1) units. In our designations

$$P_\lambda^E(\alpha \to n) = 2(2j+1)Q_\lambda^E(\alpha n;\alpha n), \qquad (4.15a)$$

$$Q_\lambda^E = Q_\lambda^{\text{Coul-Deb}} + Q_{\lambda,\lambda-1}^{Br} + Q_{\lambda,\lambda+1}^{Br}. \qquad (4.15b)$$

In a case of the two-quasi-particle states (4.for example, in a case of the Ne-like ion, where the excited state can be represented as stale with the two quasiparticles – electron and vacancy above the closed shells core $1s^22s^22p^6$) the corresponding probability has the following form (4.say, transition: $j_1 j_2[J] \to \bar{j}_1 j_2[\bar{J}]$):

$$P(\lambda \mid j_1 j_2[J], \bar{j}_1 j_2[\bar{J}]) = (\bar{J})\begin{Bmatrix} \lambda \ldots J \ldots \bar{J} \\ j_2 \ldots \bar{j}_1 \ldots j_1 \end{Bmatrix} P(\lambda \mid 1\bar{1})(\bar{j}_1), \qquad (4.16)$$

The other details of calculational procedure can be found in Refs. [39-42].The modified PC code “Superatom-ISAN” (4.version-93) has been used in all calculations.

4.3. Results and conclusions

Here we present the results of computing the radiative and collisional characteristics (energy shifts, oscillator strengths, electron-ion cross-sections and collision strengths) for the Be-, Ne-like ions of Fe, Zn and Kr embedded to the plasmas environment. It is worth to remind [13-20,29-39] that these multicharged ions play an important role in the diagnostics of a wide variety of laboratory, astrophysical, thermonuclear plasmas. Firstly, we list our results on energy shifts and oscillator strengths for transitions $2s^2$-$2s_{1/2}2p_{1/2,3/2}$ in spectra of the Be-like Ni and Kr. The plasmas parameters are as follows: $n_e=10^{22}$-$10^{24}cm^{-3}$, T=0.5-2 keV (4.i.e. μ~0.01-0.3). In tables 4.1 and 4.2 we list the results of calculation of the energy shifts ΔE ($4.cm^{-1}$) for $2s^2$-$[2s_{1/2}2p_{1/2,3/2}]_1$ transitions due to the plasmas environment effect for the Be-like multicharged ions of Kr, Fe and Zn.

Table 4.1. Energy shifts ΔE ($4.cm^{-1}$) for the $2s^2$-$[2s_{1/2}2p_{1/2,3/2}]_1$ transition in spectra of the Be-like Kr ions for different values of the n_e ($4.см^{-3}$) and T (4.in eV) (4.see explanations in text)

Z/	n_e	10^{22}	10^{23}	10^{24}	10^{22}	10^{23}	10^{24}
Transition	kT	Li et al	Li et al	Li et al	Our data	Our data	Our data
KrXXXIII	500	21.3	197.9	2191.9	27.2	215.4	2236.4
$2s^2$-	1000	15.5	150.5	1659.6	21.3	169.1	1705.1
$[2s_{1/2}2p_{3/2}]_1$	2000	11.5	113.5	1268.0	16.9	128.3	1303.8
	I-S	4.3	49.5	497.2			
KrXXXIII	500	24.8	230.7	2500.4	30.6	247.8	2545.2
$2s^2$-	1000	18.2	171.7	1893.5	24.0	188.5	1936.8
$[2s_{1/2}2p_{1/2}]_1$	2000	13.5	129.5	1446.5	18.4	144.1	1482.7
	I-S	5.4	56.4	566.3			

Table 2. Energy shifts ΔE (4.cm^{-1}) for the $2s^2$-$[2s_{1/2}2p_{1/2,3/2}]_1$ transition in spectra of the Be-like Fe and Zn ions for different values of the n_e (4.$см^{-3}$) and T (4.in eV) (4.see explanations in text)

Ion		FeXXII	FeXXIII	FeXXIII	ZnXXVII	ZnXXVII	ZnXXVII
Parameter	n_e	10^{22}	10^{23}	10^{24}	10^{22}	10^{23}	10^{24}
Transition	kT	Our data	Our data	Our data	Our data	Our data	Our data
$2s^2$-	500	31.3	344.1	3061.9	29.1	258.1	2747.6
$[2s_{1/2}2p_{3/2}]_1$	1000	23.9	264.3	2379.1	22.8	196.9	2090.2
	2000	18.8	208.5	1892.8	17.8	155.2	1634.4
$2s^2$-	500	33.5	366.9	3270.7	30.6	279.5	2994.7
$[2s_{1/2}2p_{1/2}]_1$	1000	24.9	284.2	2536.9	23.0	213.2	2273.8
	2000	19.5	222.1	2007.8	18.3	168.1	1778.1

The available theoretical data by Yongqiang Li et al and Saha-Frische (4.the multiconfiguration Dirac-Fock (4.DF) computation results and the ionic sphere (4.I-S) model simulation data from [15,16] and Refs. therein) are also presented for the Be-like ion of Kr.

Table 3. Oscillator strengths gf for the $2s^2$-$[2s_{1/2}2p_{3/2}]_1$ transition in spectra of the Be-like ion of Kr for different values of the n_e (4.$см^{-3}$) and T (4.in eV) (4.gf_0 –the gf value for free ion)

n_e		10^{22}	10^{23}	10^{24}		10^{22}	10^{23}	10^{24}
kT	gf_0 [15]	gf [15]	gf [15]	gf [15]	gf_o our data	gf our data	gf our data	gf our data
500	0.13760	0.13760	0.13763	0.13797	0.13789	0.13790	0.13812	0.13854
1000	0.13672	0.13760	0.13762	0.13788		0.13790	0.13810	0.13839
2000		0.13760	0.13762	0.13781		0.13789	0.13809	0.13824
I-S		0.13760	0.13761	0.13768				

Table 4. Oscillator strengths gf for the $2s^2$-$[2s_{1/2}2p_{3/2}]_1$ transition in spectra of the Be-like ions of Fe and Zn for different values of the n_e (4.см$^{-3}$) and T (4.in eV) (4.gf_0 –the gf value for free ion)

	Be-like ions of Fe				Be-like ions of Zn			
	n_e	10^{22}	10^{23}	10^{24}	n_e	10^{22}	10^{23}	10^{24}
kT	gf_o:our data	gf: our data	gf: our data	gf: our data	gf_o:our data	gf: our data	gf: our data	gf: our data
500	0.15403	0.15406	0.15431	0.15513	0.14354	0.14356	0.14377	0.14409
1000		0.15406	0.15428	0.15488		0.14356	0.14375	0.14396
2000		0.15404	0.15426	0.15467		0.14355	0.14373	0.14383

In tables 4.3 and 4.4 we list the results of computing oscillator strengths changes for $2s^2$-$[2s_{1/2}2p_{1/2,3/3}]_1$ transitions in spectra of the Be-like Fe and Zn ions at different plasmas parameters: the electron density n_e and temperature T. The available theoretical data on the oscillator strength changes due to the plasmas environment effect by Yongqiang Li etal [15] are also listed for the Be-like ion of Kr. The analysis shows that the presented data are in physically reasonable agreement.

However, some difference can be explained by using different relativistic orbital basis and different models for accounting of the plasmas screening effect. From the physical point of view, the behavior of the energy shift is naturally explained, i.e by increasing blue shift of the line because of the increasing the plasmas screening effect.

In table 4.5 we present the theoretical data on the effective collision strengths of the Ne-like Kr^{26+} ion excitation states for the temperature $T=5\cdot10^6$ K and the electron density $n_e=10^{14}$ cm^{-3}. The Dirac R-matrix (4.RM) calculation data by Griffin et al [28] and model potential (4.MP) data [35,36] are listed for comparison too. It should be noted that strong compensation of different PT terms is a characteristic feature of the states with vacancies in the core. This is one of the main reasons for the fact that the accuracy of conventional a priori calculations of such states does not always satisfy the requirements arising in many applications. Summation over j_{in},j_{sc} in (4.18) spreads over the range 1/2-23/2.

Table 4.5. The effective collision strengths of the Kr^{26+} Ne-like ion excitation states for the temperature $T=5\cdot10^6$ K and electron density $n_e=10^{14}$ cm^{-3} (4.see text).

Term	RM	MP	Our data
$2p^53s\ (4.3/2,1/2)_2$	8.29(4.-3)	8.13(4.-3)	8.17(4.-3)
$2p^53s\ (4.3/2,l/2)_1$	9.36(4.-3)	9.19(4.-3)	9.23(4.-3)
$2p^53p\ (4.3/2,l/2)_1$	3.49(4.-3)	3.38(4.-3)	3.41(4.-3)
$2p^53p\ (4.3/2,1/2)_2$	4.30(4.-3)	4.18(4.-3)	4.24(4.-3)
$2p^53s\ (4.1/2,l/2)_0$	1.32(4.-3)	1.21(4.-3)	1.26(4.-3)
$2p^53s\ (4.1/2,l/2)_1$	7.69(4.-3)	7.56(4.-3)	7.60(4.-3)
$2p^53p\ (4.3/2,3/2)_3$	4.03(4.-3)	3.89(4.-3)	3.94(4.-3)
$2p^53p\ (4.3/2,3/2)_1$	3.14(4.-3)	3.01(4.-3)	3.06(4.-3)
$2p^53p\ (4.3/2,3/2)_2$	3.36(4.-3)	3.12(4.-3)	3.16(4.-3)
$2p^53p\ (4.3/2,3/2)_0$	8.67(4.-3)	8.49(4.-3)	8.55(4.-3)
$2p^53p\ (4.1/2,1/2)_1$	2.69(4.-3)	2.54(4.-3)	2.59(4.-3)
$2p^53p\ (4.1/2,3/2)_1$	2.80(4.-3)	2.72(4.-3)	2.75(4.-3)
$2p^53p\ (4.1/2,3/2)_2$	3.27(4.-3)	3.16(4.-3)	3.21(4.-3)
$2p^53d\ (4.3/2,3/2)_0$	1.24(4.-3)	1.13(4.-3)	1.18(4.-3)
$2p^53p\ (4.1/2.1/2)_0$	1.71(4.-2)	1.58(4.-2)	1.63(4.-2)
$2p^53d\ (4.3/2,3/2)_1$	3.45(4.-3)	3.31(4.-3)	3.36(4.-3)
$2p^53d\ (4.3/2,3/2)_3$	3.80(4.-3)	3.67(4.-3)	3.74(4.-3)
$2p^53d\ (4.3/2,5/2)_2$	4.13(4.-3)	3.96(4.-3)	4.01(4.-3)

For some levels the corrections due the correlation effects change the results by a factor of 2-3,5. Using of the shielding approach and an accounting for the highly-lying excited states is quantitatively important for the adequate, physically reasonable description of the collision strengths. It should be noted that the experimental information about the collision strengths for high-charged Ne-like ions is very scarce and is extracted from indirect observations. Such experimental information for a few collisional excitations of the Ne-like barium ground state has been presented in Refs.[20-22].

Analysis shows that using relativistic energy approach with the optimal Dirac-Kohn-Sham one-electron PT basis and shielding model block is quite consistent and effective from the viewpoint of the theory correctness and results ex-

actness. This fact was surely confirmed by the multiple calculations of the oscillator strengths, radiative widths in atoms and multicharged ions [9,40-42,88-90,104-106].

Further we present the results of computing the radiative and collisional characteristics (energy shifts, oscillator strengths, electron-ion cross-sections and collision strengths) for the Be-, Ne-like ions of Ar, Ni and Kr (Z=18-36) embedded to the plasmas environment. Let us remind (see Ref. [11,12,16,28,39]) that the Be- and Ne-like ions play an important role in the diagnostics of a wide variety of laboratory, astrophysical, thermonuclear plasmas. Firstly, we list our results on energy shifts and oscillator strengths for transitions $2s^2$-$2s_{1/2}2p_{1/2,3/2}$ in spectra of the Be-like Ni and Kr. The plasmas parameters are as follows: $n_e=10^{22}$-$10^{24}cm^{-3}$, T=0.5-2 keV (i.e. μ~0.01-0.3). In table 4.6 and 4.7 we list the results of calculation of the energy shifts ΔE (cm^{-1}) for $2s^2$-$[2s_{1/2}2p_{1/2,3/3}]_1$ transitions and oscillator strengths changes for different plasmas parameters such as the electron density n_e and temperature T.

Table 4.6. Energy shifts ΔE (cm^{-1}) for the $2s^2$-$[2s_{1/2}2p_{3/2}]_1$ transition in spectra of the Be-like Ni and Kr ions for different values of the n_e ($см^{-3}$) and T (in eV) (see explanations in text)

	n_e	10^{22}	10^{23}	10^{24}	10^{22}	10^{23}	10^{24}
Z	kT	Li et al	Li et al	Li et al	Our data	Our data	Our data
NiXXV	500	31.3	292.8	2639.6	33.8	300.4	2655.4
	1000	23.4	221.6	2030.6	25.7	229.1	2046.1
	2000	18.0	172.0	1597.1	20.1	179.8	1612.5
	I-S	8.3	86.6	870.9			
KrXXXIII	500	21.3	197.9	2191.9	27.2	215.4	2236.4
	1000	15.5	150.5	1659.6	21.3	169.1	1705.1
	2000	11.5	113.5	1268.0	16.9	128.3	1303.8

There are also presented the available theoretical data by Li etal and Saha-Frische: the multiconfiguration Dirac-Fock (DF) computation results and ionic sphere (I-S) model simulation data (from [11,12,16] and Refs. therein). The analysis shows that the presented data are in physically reasonable agreement, however, some difference can be explained by using different relativistic orbital basis and different models for accounting of the plasmas screening effect. From the physical point of view, the behavior of the energy shift is naturally explained, i.e by increasing blue shift of the line because of the increasing the plasmas screening effect.

Table 4.6. Oscillator strengths gf for the $2s^2$-$[2s_{1/2}2p_{3/2}]_1$ transition in spectra of the Be-like ion of Ni for different values of the n_e (см$^{-3}$) and T (in eV) (gf_0 –the gf value for free ion)

n_e		10^{22}	10^{23}	10^{24}		10^{22}	10^{23}	10^{24}
kT	gf_0 Li et al	gf Li et al	gf Li et al	gf Li et al	gf_0:our data	gf: our data	gf: our data	gf: our data
500	0.1477	0.1477	0.1478	0.1487	0.1480	0.1480	0.1483	0.1495
1000		0.1477	0.1477	0.1482		0.1480	0.1483	0.1495
2000		0.1477	0.1477	0.1481		0.1479	0.1482	0.1493
I-S		0.1477	0.1477	0.1479				

Further we present the results of computing the electron-collisional cross-sections and electron-collision strengths for Ne-like ion of Ar (the part of results has been presented in Refs. [28]), but without the plasmas screening effect) and compare with the known theoretical data: relativistic model potential PT (RMPPT), relativistic optimized DF PT (ODFPT) [28-30,41,42].

In table 4.7 we list the electron-collision strengths for Ne-like argon excitation from the ground state (E=0.75 keV is the impact electron energy). The corresponding plasmas parameters (θ-pinch plasmas) are as follows: $n_e=10^{16}$ cm^{-3}, and T_e=65 eV.

Table 4.7. The electron-collision strengths for Ne-like Ar excitation from the ground state for impact electron energy 0.75 keV (numbers in brackets denote the multiplicative powers of ten)

Transition	Level	J	[41]	[29]	Present data
1-2	2s 2p	0	1,303[-03]	1,415[-03]	1,498[-03]
3	$2p_{3/2}3s_{1/2}$	1	9,017[-03]	9,224[-03]	9,286[-03]
4	$2p_{1/2}3s_{1/2}$	0	2,587[-04]	2,724[-04]	2,783[-04]
5	$2p_{1/2}3s_{1/2}$	1	2,241[-02]	2,342[-02]	2,394[-02]
6	$2p_{3/2}3p_{3/2}$	1	3,456[-03]	3,635[-03]	3,699[-03]
7	$2p_{3/2}3p_{3/2}$	3	2,911[-03]	2,998[-03]	3,065[-03]
8	$2p_{3/2}3p_{1/2}$	2	4,795[-03]	4,922[-03]	4,988[-03]
9	$2p_{3/2}3p_{1/2}$	1	1,033[-03]	1,213[-03]	1,254[-03]
10	$2p_{3/2}3p_{3/2}$	2	6,451[-03]	6,535[-03]	6,597[-03]
11	$2p_{1/2}3p_{1/2}$	1	9,641[-04]	9,993[-04]	1,088[-03]
12	$2p_{1/2}3p_{1/2}$	0	8,794[-04]	8,927[-04]	8,992[-04]
13	$2p_{1/2}3p_{3/2}$	2	7,814[-03]	7,978[-03]	8,113[-03]
14	$2p_{1/2}3p_{3/2}$	1	8,561[-04]	8,723[-04]	9,005[-04]
15	$2p_{3/2}3p_{3/2}$	0	8,670[-02]	8,735[-02]	8,802[-02]
16	$2p_{3/2}3d_{3/2}$	0	1,136[-03]	1,244[-03]	1,296[-03]
17	$2p_{3/2}3d_{3/2}$	1	4,129[-03]	4,327[-03]	4,389[-03]
18	$2p_{3/2}3d_{5/2}$	2	5,227[-03]	5,546[-03]	5,601[-03]
19	$2p_{3/2}3d_{5/2}$	4	3,512[-03]	3,678[-03]	3,714[-03]
20	$2p_{3/2}3d_{3/2}$	3	3,994[-03]	4,133[-03]	4,185[-03]

It should be noted that the experimental information about the electron-collisional cross-sections for high-charged Ne-like ions is very scarce and is extracted from indirect observations. Such experimental information for a few collisional excitations of the Ne-like barium ground state has been presented in Refs.[17-19].

Let us note that the PT first order correction is calculated exactly, the high-order contributions are taken into account for effectively: polarization interaction of two above-core quasi-particles and an effect of their mutual screening (correla-

tion effects). It is interesting to note that here the plasmas effects do not play a critical quantitative role.

Further we present the results of studying collisional characteristics for the Ne-like ions in the collisionally pumping plasmas with the parameters T_e=20-40eV and density $n_e=10^{19\text{-}20}$ cm^{-3}. This system represents a great interest for generation of laser radiation in the short-wave spectral range [3,4]. Besides, it is obviously more complicated case in comparison with previous one. Here an accurate account of the excited, Rydberg, autoionization and continuum states can play a critical role.

In table 4.8 we present the theoretical values of the collisional excitation rates (CER) and collisional de-excitation rates (CDR) for Ne-like argon transition between the Rydberg states and from the Rydberg states to the continuum states with parameters: $n_e= 10^{19\text{-}20}$ cm^{-3} and electron temperature T_e =20eV (see details in Ref. [28,42]).

For comparison there are also listed the data by Ivanov et al, obtained within the RMPPT approach (without the shielding effect) [28,41,42].

Here we talk about the Rydberg states which converge to the corresponding lower boundary of continuum $-\varepsilon_0$ (see figure 4.1).

Table 4.8 The collisional excitation (CER) and de-excitation (CDR) rates (in cm^3/s) for Ne-like argon in plasmas with parameters: $n_e= 10^{19\text{-}20}$ cm^{-3} and electron temperature T_e =20eV

Parameters	n_e, cm^{-3}	RMPPT	RMPPT	RMPPT	Present results	Present results	Present results
Transition		1→2	1→3	2→3	1→2	1→3	2→3
CDR (i→i ;k)	1.0+19	5.35-10	1.64-10	1.13-09	5.77-10	1.92-10	1.28-09
	1.0+20	5.51-10	1.60-10	1.12-09	5.94-10	1.78-10	1.25-09
Transition		2→1	3→1	3→2	2→1	3→1	3→2
CER (i→i ;k)	1.0+19	5.43-10	5.39-12	2.26-11	5.79-10	1.88-12	2.64-11
	1.0+20	3.70-10	8.32-12	2.30-11	4.85-10	1.13-11	2.78-11

As it is indicated in Ref. [42], the parameter $-\varepsilon_0$ is the third parameter of the plasmas environment (together with electron density and temperature).
In fact it defines the thermalized energy zone of the Rydberg and autoionization states which converge to the ionization threshold for each ion in a plasmas. Usually value ε_0 can be barely estimated from simple relation: $\varepsilon_0 = 0.1 \cdot T_e$.

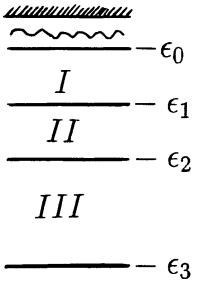

Figure 4.1. The Rydberg states zones (Ne-like ion: [Ne,i], nl); ε_0 is the boundary of the thermalized zone, neighboring to continuum; ε_3 is the ionization potential for states $nl=3s$; $\varepsilon_i=(\varepsilon_0+\varepsilon_{i+1})/2$, i=1,2;

In the consistent theory the final results must not be dependent on the model parameters, so the concrete value of ε_0 is usually chosen in such way that an effect of its variation in the limits $[0.01 \cdot T_e , 0.1 \cdot T_e]$ (for Ne-like ions) does not influence on the final results.

In table 4.9 we present the theoretical values of the collisional excitation (CER) and de-excitation (CDR) rates (in cm^3/s) for Ne-like argon in plasmas with the parameters: $n_e = 10^{19\text{-}20}\ cm^{-3}$ and electron temperature T_e = 40 eV. Analysis of the presented data allows to conclude that the shielding effects play a definite role for the Debye plasmas.

From other side, an account for the highly-lying excited states is quantitatively important for the adequate description of the collision cross-sections.

Table 4.9. The collisional excitation (CER) and de-excitation (CDR) rates (in cm^3/s) for Ne-like argon in plasmas with parameters: $n_e = 10^{19-20}$ cm^{-3} and electron temperature T_e =40eV (our data)

Parameters	n_e, cm^{-3}	Present results	Present results	Present results
Transition		1→2	1→3	2→3
CDR (i→i ;k)	1.0+19	3.18-10	8.45-11	6.81-10
	1.0+20	5.02-10	1.56-10	4.99-10
Transition		2→1	3→1	3→2
CER (i→i ;k)	1.0+19	5.33-10	5.63-10	7.11-11
	1.0+20	7.67-10	6.94-11	8.93-11

The calculations encourage us to believe that using energy approach combined with the relativistic many-body PT with the optimal one-electron basis is quite consistent and effective tool from the point of view of the theory correctness and results exactness. This fact was surely confirmed by other calculations of the oscillator strengths, radiative widths, hyperfine structure constants for atoms and multicharged ions (see Refs. [28-30, 49-54]).

To conclude, we have presented an effective quantum approach in radiative and collisional spectroscopy of the multicharged ions in plasmas to compute the important radiative and elementary collisional process characteristics. It is based on the generalized relativistic energy approach and relativistic optimized many-body PT with the Debye shielding model Hamiltonian for electron-nuclear and electron-electron systems. The approach is universal and, generally speaking, can be applied to quantum systems of other nature. Its application is especially perspective when the experimental information about corresponding properties and systems is very scarce. We have presented some calculation results on oscillator and effective collision strengths for the Be-and Ne-like ions of Kr, Fe and Zn in plasmas. The obtained data can be used in different applications, namely, in astrophysical analysis, laboratory, thermonuclear plasmas diagnostics, fusion research, laser physics, quantum electronics etc.

4.4. References

1. Oks, E. Spectral Line Shapes in Plasmas and Gases; Oks, E., Dalimier, E., Stamm, R., Stehle, C., Gonzalez, M.A., Eds.; Int. J. Spectr. **2010,** 1, 852581.
2. Griem, H.R. Spectral Line Broadening by Plasmas. Academic Press. New York, **1974**.
3. Ivanova, E.P. Highly efficient tabletop x-ray laser at λ=41.8 nm in Pd-like xenon pumped by optical-field ionization in a cluster jet. Phys. Rev. A. **2011,** 84, 043829.
4. Ivanova, E.P.; Grant, I.P. Oscillator strength anomalies in the neon isoelectronic sequence with applications to x-ray laser modeling. J. Phys.B: At. Mol. Opt. Phys. **1998,** 31, 2871-2880.
5. Malinovskaya, S.V.; Glushkov, A.V. Calculation of the spectra of potassium-like multicharged ions. Russian Phys. Journal. **1992,** 35(4.11), 999-1004.
6. Ignatenko, A.V. Probabilities of the radiative transitions between Stark sublevels in spectrum of atom in an DC electric field: New approach. Photoelectronics, **2007,** 16, 71-74.
7. Glushkov, A.V.; Ambrosov, S.V.; Ignatenko, A.V. Non-hydrogenic atoms and Wannier-Mott excitons in a DC electric field: Photoionization, Stark effect, Resonances in ionization continuum and stochasticity. Photoelectronics, **2001,** 10, 103-106.
8. Glushkov, A.V.; Loboda, A.V.; Gurnitskaya, E.P.; Svinarenko, A.A. QED theory of radiation emission and absorption lines for atoms in a strong laser field. Phys. Scripta. **2009,** T135, 014022.
9. Glushkov, A.V.; Khetselius, O.Yu.; Svinarenko, A.A. Theoretical spectroscopy of autoionization resonances in spectra of lanthanide atoms. Phys. Scripta. **2013**, T153, 014029.
10. Burke, P.G.; Robb, W.D. The R-Matrix Theory of Atomic Processes. Adv. in Atom. and Mol. Phys. **1976,** 11, 143-214.
11. Witthoeft, M.C.; Whiteford, A.D.; Badnell N.R. R-matrix electron-impact excitation calculations along the F-like iso-electronic sequence. J. Phys. B: At. Mol. Opt. Phys. **2007,** 40, 2969-2994.
12. Liang, G.Y.; Badnell, N.R. R-matrix electron-impact excitation data for

the Ne-like iso-electronic sequence. Astr. &Astrophys. **2010,** A518, A64.

13. Paul, S.; Ho, Y.K. Two-colour three-photon transitions in a hydrogen atom embedded in Debye plasmas. J. Phys. B: At. Mol. Opt. Phys. **2010,** 43, 065701.
14. Kar, S.; Ho, Y.K. Resonances in electron–hydrogen scattering in Debye plasmas. J. Phys. B: At. Mol. Opt. Phys. **2011,** 44, 015001.
15. Yongqiang, Li; Jianhua, Wu; Yong, Hou, Jianmin Yuan. Influence of hot and dense plasmas on energy levels and oscillator strengths of ions: Be-like ions for Z = 26–36, J. Phys. B: At. Mol. Opt. Phys. **2008,** 41, 145002.
16. Saha B.; Fritzsche S. Influence of dense plasma on the low-lying transitions in Be-like ions: relativistic multiconfiguration Dirac–Fock calculation. J. Phys. B: At. Mol. Opt. Phys. **2007,** 40, 259-270.
17. Das, M.; Chaudhuri, R.K.; Chattopadhyay, S. Application of relativistic Fock-space coupled-cluster theory to study Li and Li-like ions in plasma. Phys. Rev. A. **2012,** 85(4.4), 042506.
18. Das, M.; Sahoo, B.K.; Pal, S. Plasma screening effects on the electronic structure of multiply charged Al ions using Debye and ion-sphere models. Phys. Rev. A. **2016,** 93 (4.5), 052513
19. Sahoo, B.K.; Das, M. Plasma-screening effects in the astrophysically relevant He-like and Li-like Mg and Fe ions. Eur. Phys. J. D **2016,** 70, 270-280.
20. Marrs, R.; Levine, M.; Knapp, D.; Henderson, J. Measurement of electron-impact–excitation cross sections for very highly charged ions. Phys. Rev. Lett. **1988,** 60, 1715-1719.
21. Zhang, H.; Sampson, D.; Clark, R.; Mann, J. Collision strengths and oscillator strengths for excitation to the n = 3 and 4 levels of neon-like ions. At. Data Nuc. Data Tabl. **1988,** 37, 17-51.
22. Reed, K.J. Relativistic distorted-wave collision strengths for Ba^{46+}. Phys. Rev. A. **1988,** 37, 1791-1794.
23. Smith, A.C.H.; Bannister, M.E.; Chung, Y.-S.; Djuric, N.; Dunn, G.H.; Wallbank, B.; Woitke, O. Near-threshold Electron-impact Excitation of Multiply-charged Be-like Ions. Phys. Scripta. **1999,** 80, 283-284.
24. Svinarenko, A.A. Study of spectra for lanthanides atoms with relativistic many- body perturbation theory: Rydberg resonances. J. Phys.: Conf. Ser.

2014, 548, 012039.

25. Okutsu, H.; Sako, T.; Yamanouchi, K.; Diercksen, G.H.F. Electronic structure of atoms in laser plasmas: Debae shielding approach. J. Phys. B: At. Mol. Opt. Phys. **2005,** 38, 917-927
26. Nakamura, N.; Kavanagh, A.P.; Watanabe, H.; Sakaue, H.A.; Li, Y.; Kato, D.; Curell, F.J.; Ohtani, S. Relativistic effects on resonant interactions between electrons and highly charged ions. J.Phys.: Conf. Ser. **2007,** 88, 012066.
27. Bannister, M.E.; Djuric, N.; Woitke, O.; Dunn, G.H.; Chung, Y.-S.; Smith, A.C.H.; Wallbank, B.; Berrington, K.A. Absolute cross sections for near-threshold electron-impact excitation of Be-like C^{2+}, N^{3+}, and O^{4+} ions. Int. Journ. Mass Spectr. **1999,** 192, 39-48.
28. Griffin, D.C.; Balance, C.P.; Mitnik, D.M.; Berengut, J.C. Dirac R–matrix calculations of electron–impact excitation of neon–like krypton. J. Phys. B: At. Mol. Opt. Phys. **2008,** 41, 215201.
29. Badnell, N.R. Calculations for electron-ion collisions and photoionization processes for plasma modeling. J.Phys.: Conf. Ser. **2007,** 88, 012070.
30. Ivanov, L.N.; Ivanova, E.P.; Knight, L.; Molchanov, A.G. Spectrum of plasma containing Ne- and Na-like ions: consistent account for Rydberg and autoionizing Rydberg series in balance equations. Phys.Scripta. **1996,** 53, 653-667.
31. Glushkov, A.V.; Malinovskaya, S.V.; Gurnitskaya, E.P.; Khetselius, O.Yu.; Dubrovskaya, Yu.V. Consistent quantum theory of recoil induced excitation and ionization in atoms during capture of neutron. J. Phys.: Conf. Ser. **2006,** 35, 425-430.
32. Glushkov, A.V.; Malinovskaya, S.V.; Prepelitsa, G.P.; Ignatenko, V. Manifestation of the new laser-electron nuclear spectral effects in the thermalized plasma: QED theory of co-operative laser-electron-nuclear processes. J. Phys.: Conf. Ser. **2005,** 11, 199-206.
33. Glushkov, A.V.; Malinovskaya, S.V.; Chernyakova Y.G.; Svinarenko, A.A. Cooperative laser-electron-nuclear processes: QED calculation of electron satellites spectra for multi-charged ion in laser field. Int. Journ. Quant. Chem. **2004,** 99, 889-893.
34. Glushkov, A.V.; Malinovskaya, S.V.; Loboda, A.V.; Shpinareva, I.M.;

Gurnitskaya, E.P.; Korchevsky, D.A. Diagnostics of the collisionally pumped plasma and search of the optimal plasma parameters of x-ray lasing: calculation of electron-collision strengths and rate coefficients for Ne-like plasma. J. Phys.: Conf. Ser. **2005,** 11, 188-198.

35. Glushkov, A.V.; Ambrosov, S.V.; Loboda, A.V.; Gurnitskaya, E.P.; Prepelitsa, G.P. Consistent QED approach to calculation of electron-collision excitation cross sections and strengths: Ne-like ions. Int. J. Quantum Chem. **2005,** 104, 562-569.
36. Glushkov, A.V.; Khetselius, O.Yu.; Loboda, A.V.; Ignatenko, A.V.; Svinarenko, A.A.; Korchevsky, D.A.; Lovett, L. QED approach to modeling spectra of the multicharged ions in a plasma: oscillator and electron-ion collision strengths. AIP Conf. Proceedings. **2008,** 1058, 175-177.
37. Ivanov, L.N.; Ivanova, E.P.; Aglitsky, E.V. Modern trends in the spectroscopy of multicharged ions. Phys. Rep. **1988,** 166, 315-390.
38. Ivanov, L.N.; Ivanova, E.P. Method of Sturm orbitals in calculation of physical characteristics of radiation from atoms and ions. JETP. **1996,** 83, 258-266.
39. Buyadzhi, V.V.; Zaichko, P.A.; Antoshkina, O.A.; Kulakli, T.A.; Prepelitsa, G.P.; Ternovsky V.B.; Mansarliysky, V.F. Computing of radiation parameters for atoms and multicharged ions within relativistic energy approach: Advanced Code. J. Phys.: Conf. Ser. **2017,** 905, 012003.
40. Buyadzhi, V.V. Laser multiphoton spectroscopy of atom embedded in Debye plasmas: multiphoton resonances and transitions. Photoelectronics. **2015,** 24, 128-133.
41. Buyadzhi, V.V.; Chernyakova, Yu.G.; Smirnov, A.V.; Tkach, T.B. Electron-collisional spectroscopy of atoms and ions in plasma: Be-like ions. Photoelectronics. **2016,** 25, 97-101.
42. Buyadzhi, V.V.; Chernyakova, Yu.G.; Antoshkina, O.A.; Tkach, T.B. Spectroscopy of multicharged ions in plasmas: Oscillator strengths of Be-like ion Fe. Photoelectronics. **2017,** 26, 94-102.
43. Ivanov, L.N.; Ivanova, E.P. Atomic ion energies for Na-like ions by a model potential method Z = 25–80. Atom. Data Nucl. Data Tabl. **1979,** 24, 95-109.
44. Driker, M.N.; Ivanova, E.P.; Ivanov, L.N.; Shestakov, A.F. Relativistic

calculation of spectra of 2-2 transitions in O-and F-like atomic ions. J.Quant.Spectr. Rad. Transfer. **1982,** 28, 531-535.

45. Vidolova-Angelova, E.; Ivanov, L.N.; Ivanova, E.P.; Angelov, D.A. Relativistic perturbation theory method for investigating the radiation decay of highly excited many electron atomic states. Application to the Tm atom. J. Phys. B: At. Mol. Opt. Phys. **1986,** 19, 2053-2069.
46. Ivanova, E.P.; Gulov, A.V. Theoretical investigation of the neon isoelectronic sequence. Atom. Data Nuc. Data Tabl. **1991,** 49, 1-64.
47. Ivanova, E.P.; Ivanov, L.N.; Glushkov, A.V.; Kramida, A.E. High order corrections in the relativistic perturbation theory with the model zeroth approximation, Mg-Like and Ne-Like Ions. Phys. Scripta 1985, 32, 513-522.
48. Ivanov, L.N.; Letokhov, V.S. Doubly excited autoionization states of multielectron atoms. Com.Mod.Phys.D.:At.Mol.Phys. **1985,** 4, 169-184.
49. Ivanova, E.P.; Glushkov, A.V. Theoretical investigation of spectra of multicharged ions of F-like and Ne-like isoelectronic sequences. J. Quant. Spectr. Rad. Transfer. 1986, 36, 127-145.
50. Ivanov, L.N.; Ivanova, E.P.; Knight, L. Energy approach to consistent QED theory for calculation of electron-collision strengths: Ne-like ions. Phys. Rev. A. **1993,** 48, 4365-4374.
51. Glushkov, A.V.; Ivanov, L.N.; Ivanova, E.P. Autoionization Phenomena in Atoms. Moscow University Press, Moscow, **1986,** 58-160
52. Glushkov, A.V.; Ivanov, L.N. Radiation decay of atomic states: atomic residue polarization and gauge noninvariant contributions. Phys. Lett. A **1992,** 170, 33-36.
53. Glushkov, A.V. Relativistic Quantum theory. Quantum mechanics of atomic systems; Astroprint: Odessa, **2008**.
54. Glushkov, A.V. Energy approach to resonance states of compound superheavy nucleus and EPPP in heavy nuclei collisions In Low Energy Antiproton Physics; Grzonka, D., Czyzykiewicz, R., Oelert,W., Rozek, T., Winter, P., Eds.; AIP: New York, AIP Conf. Proc. **2005**, 796, 206-210.
55. Glushkov, A.V. Spectroscopy of cooperative muon-gamma-nuclear processes: Energy and spectral parameters J. Phys.: Conf. Ser. **2012,** 397, 012011

56. Glushkov, A.V. Advanced Relativistic Energy Approach to Radiative Decay Processes in Multielectron Atoms and Multicharged Ions. In Quantum Systems in Chemistry and Physics: Progress in Methods and Applications, Series: Progress in Theoretical Chemistry and Physics; Nishikawa, K., Maruani, J., Brändas, E., Delgado-Barrio, G., Piecuch, P., Eds.; Springer: Dordrecht, **2012**; Vol. 26, pp 231–252.
57. Glushkov, A.V. Spectroscopy of atom and nucleus in a strong laser field: Stark effect and multiphoton resonances. J. Phys.: Conf. Ser. **2014**, 548, 012020
58. Khetselius, O.Yu. Spectroscopy of cooperative electron-gamma-nuclear processes in heavy atoms: NEET effect. J. Phys.: Conf. Ser. **2012,** 397, 012012.
59. Khetselius, O.Yu. Relativistic Energy Approach to Cooperative Electron-γ-Nuclear Processes: NEET Effect In Quantum Systems in Chemistry and Physics, Series: Progress in Theoretical Chemistry and Physics; Nishikawa, K., Maruani, J., Brändas, E., Delgado-Barrio, G., Piecuch, P., Eds.; Springer: Dordrecht, **2012;** Vol. 26, pp 217-229.
60. Khetselius, O.Yu. Hyperfine structure of atomic spectra. Astroprint: Odessa, **2008**.
61. Glushkov A.V.; Ivanov, L.N. DC strong-field Stark effect: consistent quantum-mechanical approach. J. Phys. B: At. Mol. Opt. Phys. **1993,** 26, L379-386.
62. Glushkov, A.V. Oscillator strengths of Cs and Rb-like ions. Journ. of Applied Spectroscopy. **1992**, 56(4.1), 5-9
63. Glushkov, A.V. Relativistic polarization potential of a many-electron atom. Soviet Phys. Journ. **1990**, 33(4.1), 1-4.
64. Glushkov, A.V. Negative ions of inert gases. JETP Lett. **1992,** 55, 97-100.
65. Glushkov, A.V. Operator Perturbation Theory for Atomic Systems in a Strong DC Electric Field. In Advances in Quantum Methods and Applications in Chemistry, Physics, and Biology, Series: Progress in Theoretical Chemistry and Physics; Hotokka, M., Brändas, E., Maruani, J., Delgado-Barrio, G., Eds.; Springer: Cham, **2013**; Vol. 27, pp 161–177.
66. Glushkov, A.V.; Ambrosov, S.A.; Loboda, A.V.; Gurnitskaya, E.P.; Khetselius, O.Yu. QED calculation of heavy multicharged ions with ac-

count for correlation, radiative and nuclear effects. In Recent Advances in the Theory of Chemical and Physical Systems, Series: Progress in Theoretical Chemistry and Physics; Julien, P., Maruani, J., Mayou, D., Wilson, S., Delgado-Barrio, G., Eds.; Springer: Dordrecht, **2006**; Vol.15, pp 285–299.

67. Khetselius, O.Yu. Quantum structure of electroweak interaction in heavy finite Fermi-systems. Astroprint: Odessa, **2011**.
68. Malinovskaya, S.V.; Glushkov, A.V.; Khetselius, O.Y. New Laser-Electron Nuclear Effects in the Nuclear γ Transition Spectra in Atomic and Molecular Systems. In Frontiers in Quantum Systems in Chemistry and Physics, Series: Progress in Theoretical Chemistry and Physics; Wilson, S., Grout, P., Maruani, J., Delgado-Barrio, G., Piecuch, P., Eds.; Springer: Dordrecht, **2008;** Vol. 18, pp 525-541.
69. Glushkov, A.V.; Khetselius, O.Yu.; Malinovskaya, S.V. Optics and spectroscopy of cooperative laser-electron nuclear processes in atomic and molecular systems – new trend in quantum optics. Europ. Phys. Journ. ST **2008,** 160, 195-204.
70. Glushkov, A.V.; Khetselius, O.Yu.; Malinovskaya, S.V. Spectroscopy of cooperative laser–electron nuclear effects in multiatomic molecules. Molec. Phys. **2008,** 106, 1257-1260.
71. Glushkov, A.V.; Khetselius, O.Yu.; Svinarenko, A.A. Relativistic theory of cooperative muon-γ -nuclear processes: Negative muon capture and metastable nucleus discharge. In Advances in the Theory of Quantum Systems in Chemistry and Physics, Series: Progress in Theoretical Chemistry and Physics; Hoggan, P., Brändas, E., Maruani, J., Delgado-Barrio, G., Piecuch, P. Eds.; Springer: Dordrecht, **2012**; Vol. 22, pp 51–68.
72. Glushkov, A.V.; Khetselius, O.Yu.; Lovett, L. Electron-β-Nuclear Spectroscopy of Atoms and Molecules and Chemical Bond Effect on the β-Decay Parameters. In Advances in the Theory of Atomic and Molecular Systems Dynamics, Spectroscopy, Clusters, and Nanostructures, Series: Progress in Theoretical Chemistry and Physics; Piecuch, P., Maruani, J., Delgado-Barrio, G., Wilson, S., Eds.; Springer: Dordrecht, **2009**; Vol. 20, pp 125–152.
73. Glushkov, A.V.; Khetselius, O.Yu.; Loboda, A.V.; Svinarenko, A.A.

QED approach to atoms in a laser field: Multi-photon resonances and above threshold ionization In Frontiers in Quantum Systems in Chemistry and Physics, Series: Progress in Theoretical Chemistry and Physics; Wilson, S., Grout, P., Maruani, J., Delgado-Barrio, G., Piecuch, P., Eds.; Springer: Dordrecht, **2008;** Vol. 18, pp 543-560.

74. Glushkov, A.V.; Khetselius, O.Yu.; Svinarenko, A.A.; Prepelitsa, G.P.; Shakhman, A.N. Spectroscopy of Cooperative Laser-Electron Nuclear processes in Diatomic and Multiatomic Molecules. AIP Conf. Proceedings. **2010,** 1290(4.1), 269-273.
75. Glushkov, A.V.; Khetselius, O.Yu.; Lopatkin, Yu.M.; Florko, T.A.; Kovalenko, O.A.; Mansarliysky, V.F. Collisional shift of hyperfine line for rubidium in an atmosphere of the buffer inert gas. J. Phys.: Conf. Ser. **2014,** 548, 012026
76. Khetselius, O.Yu. Relativistic Hyperfine Structure Spectral Lines and Atomic Parity Non-conservation Effect in Heavy Atomic Systems within QED Theory. AIP Conf. Proceedings. **2010,** 1290(4.1), 29-33.
77. Glushkov, A.V.; Rusov, V.D.; Ambrosov, S.V.; Loboda, A.V. Resonance states of compound super-heavy nucleus and EPPP in heavy nucleus collisions In New Projects and New Lines of Research in Nuclear Physics. Fazio, G., Hanappe, F., Eds.; World Scientific: Singapore, **2003**, 126-132.
78. Glushkov, A.V.; Khetselius, O.Yu.; Gurnitskaya, E.P.; Loboda, A.V.; Florko, T.A.; Sukharev, D.E.; Lovett, L. Gauge-Invariant QED perturbation theory approach to calculating nuclear electric quadrupole moments, hyperfine structure constants for heavy atoms and ions In Frontiers in Quantum Systems in Chemistry and Physics, Series: Progress in Theoretical Chemistry and Physics; Wilson, S., Grout, P., Maruani, J., Delgado-Barrio, G., Piecuch, P., Eds.; Springer: Dordrecht, **2008;** Vol. 18, pp 507-524.
79. Glushkov, A.V.; Ambrosov, S.V.; Loboda, A.V.; Chernyakova, Yu.G.; Svinarenko, A.A.; Khetselius, O.Yu. QED calculation of the superheavy elements ions: Energy levels, Lamb shift, hyperfine structure, nuclear finite size effect. Nucl. Phys. A.: Nucl. and Hadr. Phys. **2004,** 734S, E21-E24.
80. Glushkov, A.V.; Efimov, V.A.; Gopchenko, E.D.; Dan'kov, S.V.;

Polishchyuk, V.N.; Goloshchak, O.P. Calculation of spectroscopic characteristics 4 of alkali-metal dimers on the basis of a model perturbation theory. Optics and Spectr. **1998,** 84(4.5), 670-678.

81. Khetselius, O.Yu. Relativistic Calculating the Spectral Lines Hyperfine Structure Parameters for Heavy Ions. AIP Conf. Proc. **2008,** 1058, 363-365.
82. Glushkov, A.V.; Ambrosov, S.V.; Ignatenko, A.V.; Korchevsky, D.A. DC strong field stark effect for nonhydrogenic atoms: Consistent quantum mechanical approach. Int. Journ. Quant. Chem. **2004,** 99, 936-939.
83. Glushkov, A.V.; Malinovskaya, S.V.; Sukharev, D.E.; Khetselius, O.Yu.; Loboda, A.V.; Lovett, L. Green's function method in quantum chemistry: New numerical algorithm for the Dirac equation with complex energy and Fermi-model nuclear potential. Int. Journ.Quant.Chem. 2009, 109, 1717-1727.
84. Khetselius, O.Yu. Relativistic perturbation theory calculation of the hyperfine structure parameters for some heavy-element isotopes. Int. Journ.Quant.Chem. **2009,** 109, 3330-3335.
85. Khetselius, O.Yu. Relativistic calculation of the hyperfine structure parameters for heavy elements and laser detection of the heavy isotopes. Phys.Scripta. **2009,** 135, 014023.
86. Glushkov, A.V.; Lovett, L.; Khetselius, O.Yu.; Gurnitskaya, E.P.; Dubrovskaya, Yu.V.; Loboda, A.V. Generalized multiconfiguration model of decay of multipole giant resonances applied to analysis of reaction (4.μ - n) on the nucleus ^{40}Ca. Int. J. Modern Phys. A. **2009,** 24(4.2-3), 611-615
87. Glushkov, A.V.; Malinovskaya, S.V.; Loboda, A.V.; Shpinareva, I.M.; Prepelitsa, G.P. Consistent quantum approach to new laser-electron-nuclear effects in diatomic molecules. J.Phys.: Conf. Ser. **2006,** 35, 420-424.
88. Glushkov, A.V.; Mansarliysky, V.F.; Khetselius, O.Yu.; Ignatenko, A.V.; Smirnov, A.; Prepelitsa, G.P. Collisional shift of hyperfine line for thallium in an atmosphere of the buffer inert gases. J. Phys.: Conf. Ser. **2017,** 810, 012034.
89. Glushkov, A.V.; Loboda, A.V. Calculation of the characteristics of radia-

tive multiphoton absorption and emission lines when an atom interacts with pulsed laser radiation. J. Appl.Spectr.(4.Springer). **2007,** 74, 305-309.

90. Buyadzhi, V.V.; Zaichko, P.A.; Gurskaya, M.Y.; Kuznetsova, A.A.; Ponomarenko E.L.; Ternovsky, V.B.; Relativistic theory of excitation and ionization of Rydberg atomic systems in a Black-body radiation field, J. Phys.: Conf. Ser. **2017,** 810, 012047
91. Prepelitsa, G.P.; Buyadzhi, V.V.; Ternovsky, V.B. Non-linear analysis of chaotic self-oscillations in backward-wave tube. Photoelectronics, **2013,** 22,103-107.
92. Khetselius, O.Yu. On possibility of sensing nuclei of the rare isotopes by means of laser spectroscopy of hyperfine structure, Sensor Electr. and Microsyst. Techn. **2008,** 3, 28-33.
93. Glushkov, A.V.; Khetselius, O.; Gurnitskaya, E.; Loboda, A.; Sukharev, D. Relativistic quantum chemistry of heavy ions and hadronic atomic systems: Spectra and energy shifts, AIP Conference Proceedings **2009,** 1102 (4.1), 168-171.
94. Löwdin, Per-Olov; Shull, H. Natural Orbitals in the quantum theory of two-electron systems Phys. Rev. 1956, 101, 1730
95. Feller, D.; Davidson, E.R. An approximation to frozen natural orbitals through the use of the Hartree–Fock exchange potential. J. Chem. Phys. **1981,** 74, 3977.
96. Froelich, P.; Davidson, E.R.; Brändas, E. Error estimates for complex eigenvalues of dilated Schrödinger operators. Phys. Rev. A **1983,** 28, 2641.
97. Rittby, M.; Elander, N.; Brändas, E. Scattering in view of the Titchmarsh–Weyl theory. Int. J. Quant. Chem. **1983,** 23, 865-874.
98. Maruani, J. The Dirac Electron: From Quantum Chemistry to Holistic Cosmology. Chin. J. Chem.Soc. **2016,** 63,33-48.
99. Pavlov, R.; Mihailov, L.; Velchev, Ch.; Dimitrova-Ivanovich, M.; Stoyanov, Zh.; Chamel, N.; Maruani, J. Effects induced by nuclear deformations and electron correlations on the ground-state energy of low and multiply charged helium like ions in high-temperature plasmas. J.Phys.: Conf. Ser. **2010,** 253, 012075.
100. Glushkov, A.V.; Khetselius, O.Yu.; Svinarenko, A.A.; Prepelitsa,

G.P.; Mischenko, E.V. The Green's Functions and Density Functional Approach to Vibrational Structure in the Photoelectron Spectra for Molecules, AIP Conf. Proc.**2010,** 1290, 263-268.

101. Glushkov, A.V. Relativistic multiconfiguration time-dependent self-consistent-field theory for molecules. Sov. Phys. Journal. **1991**, 34(4.10), 871-876.
102. Glushkov, A.V.; Efimov, V.A.; Gopchenko, E.D.; Dan'kov, S.V.; Polishchyuk, V.N.; Goloshchak, O.P. Calculation of spectroscopic characteristics of alkali-metal dimers on the basis of a model perturbation theory. Optika i Spektr. **1998,** 84(4.5), 747.
103. Glushkov, A.V.; Malinovskii, A.V.; Efimov, V.A.; Kivganov, A.F.; Khokhlov, V.N.; Vitavetskaya, L.A.; Borovskaya, G.A. Calculation of alkaline metal dimers in terms of model perturbation theory. J. Struct. Chem. **1988,** 39(4.2), 179-185.
104. Khetselius, O.Yu. Optimized Perturbation Theory for Calculating the Hyperfine Line Shift and Broadening of Heavy Atoms in a Buffer Gas. In Frontiers in Quantum Methods and Applications in Chemistry and Physics, Series: Progress in Theoretical Chemistry and Physics; Nascimento, M., Maruani, J., Brändas, E., Delgado-Barrio, G., Eds.; Springer: Cham, **2015;** Vol. 29, pp 55-76.
105. Khetselius, O.Yu.; Glushkov, A.V.; Gurnitskaya, E.P.; Loboda, A.V.; Mischenko, E.V.; Florko, T.; Sukharev, D. Collisional Shift of the Tl Hyperfine Lines in Atmosphere of Inert Gases. AIP Conf. Proc. **2008,** 1058, 231-233.
106. Khetselius, O.Yu. Hyperfine structure of energy levels for isotopes ^{73}Ge, ^{75}As, ^{201}Hg. Photoelectronics. **2007,** 16, 129-132.
107. Khetselius, O.Yu.; Gurnitskaya, E.P. Sensing the electric and magnetic moments of a nucleus in the N-like ion of Bi. Sensor Electr. and Microsyst. Techn. **2006,** 3, 35-39.
108. Khetselius O.Yu.; Gurnitskaya, E.P. Sensing the hyperfine structure and nuclear quadrupole moment for radium. Sensor Electr. and Microsyst. Techn. **2006,** 2, 25-29.
109. Kohn, J.W.; Sham, L.J. Self-Consistent Equations Including Exchange and Correlation Effects. Phys. Rev. A **1964,** 140, 1133.

110. Hohenberg, P.; Kohn, W. Inhomogeneous Electron Gas. Phys. Rev. B **1964,** 136, 864.
111. Glushkov, A.V. True effective molecular valency hamiltonian in a logical semiempricial theory. Journal of Structural Chem. **1988**, 29(4.4), 495-501.
112. Glushkov, A.V. Correction for exchange and correlation effects in multielectron system theory. Journal of Structural Chem. **1990**, 31(4.4), 529-532.
113. Glushkov, A.V. Polarization effects in ethylene molecule spectrum calculation. Journal of Appl. Spectroscopy. **1992,** 56 (4.3), 309–312.
114. Glushkov, A.V. New form of effective potential to calculate polarization effects of the π-electronic states of organic molecules, J. Struct. Chem. **1994**, 34, 659–665.
115. Glushkov, A.V.; Antonenko, T.N.; Serbov, N.G.; Ambrosov, S.V.; Orlova, V.E.; Orlov, S.V.; Dormostuchenko, G.M.; Chernyshova, A.K. Transition energies and oscillator strengths in the spectrum of a CO molecule. Journ. of Applied Spectrosc. **1996,** 63 (4.2), 279-282.
116. Glushkov, A.V. QED theory of radiation emission and absorption lines for atoms and ions in a strong laser field. AIP Conf. Proc. **2008,** 1058, 134-136.
117. Glushkov, A.V.; Kondratenko, P.A.; Lepikh, Y.I.; Fedchuk, A.P.; Lovett, L.; Svinarenko, A.A. Electrodynamical and quantum-chemical approaches to modeling the electrochemical and catalytic processes on metals, metal alloys, and semiconductors. Int. Journ. Quant. Chem. **2009,** 109(4.14), 3473-3481.
118. Khetselius, O.Yu. Atomic parity non-conservation effect in heavy atoms and observing P and PT violation using NMR shift in a laser beam: To precise theory. J. Phys.: Conf. Ser. **2009,** 194, 022009.
119. Glushkov, A.V.; Malinovskaya, S.V.; Filatov, V.V. S-Matrix formalism calculation of atomic transition probabilities with inclusion of polarization effects. Sov. Phys. Journal. **1989,** 32(4.12), 1010-1014.
120. Glushkov, A.V.; Butenko, Yu.V.; Serbov, N.G.; Ambrosov, S.V.; Orlova, V.E.; Orlov, S.V.; Balan, A.K.; Dormostuchenko, G.M. Calculation of the oscillator strengths in Fr-like multiply charged ions. Journ. of Applied

Spectrosc. **1996,** 63(4.1), 28-30.
121. Glushkov, A.V.; Butenko, Yu.V.; Serbov, N.G.; Ambrosov, S.V.; Orlova, V.E.; Orlov, S.V.; Balan, A.K.; Dormostuchenko, G.M. Calculation and extrapolation of oscillator strengths in Rb-like, multiply charged ions. Russian Phys. Journ. **1996**, 39(4.1), 81-83.
122. Dietz, K.; Heβ, B.A. Single particle orbitals for configuration interaction derived from quantum electrodynamics. Phys. Scripta. **1989,** 39, 682-688.
123. The Fundamentals of Electron Density, Density Matrix and Density Functional Theory in Atoms, Molecules and the Solid State, Series: Progress in Theoretical Chemistry and Physics. Gidopoulos, N. and Wilson, S., Eds.; Springer: Dordrecht, **2004**.
124. Malinovskaya, S.V.; Dubrovskaya, Yu.V.; Vitavetskaya, L.A. Advanced quantum mechanical calculation of the beta decay probabilities. AIP Conf. Proc. **2005**, 796, 201-205.
125. Glushkov, A.V. Relativistic and Correlation Effects in Spectra of Atomic Systems. Astroprint: Odessa, **2006**.
126. Malinovskaya, S.V.; Glushkov, A.V.; Khetselius, O.Yu.; Svinarenko, A.A.; Mischenko, E.V.; Florko, T.A. Optimized perturbation theory scheme for calculating the interatomic potentials and hyperfine lines shift for heavy atoms in the buffer inert gas. Int. J. Quant. Chem. **2009,** 109(4.4), 3325-3329.
127. Zeng, S.L.; Liu, L.; Wang, J.G.; Janev, R.K. Atomic collisions with screened Coulomb interactions: excitation and electron capture in $H^+ + H$ collisions. J. Phys. B: At. Mol. Opt. Phys. **2008,** 41, 135202.
128. Filatov, M.; Cremer, D. A gauge-independent zeroth-order regular approximation to the exact relativistic Hamiltonian—Formulation and applications. J. Chem. Phys. **2005**, 122, 044104.
129. Wang, Y.A.; Yung, Y.C.; Chen, Y.K.; Chen, G.H. Communication: Linear-expansion shooting techniques for accelerating self-consistent field convergence. J. Chem. Phys. **2011,** 134, 241103.
130. Suaud N.; Malrieu, J.-P. Natural molecular orbitals: limits of a Lowdin's conjecture, Mol. Phys. **2017**, 115(4.21-22), 2684-2695.

CHAPTER 5. HYPERFINE AND ELECTROWEAK INTERACTION IN HEAVY FINITE FERMI-SYSTEMS AND PARITY NON-CONSERVATION EFFECT

5. 1 Introduction

The consistent theoretical approach, namely, nuclear-relativistic many-body perturbation theory is applied to study of the hyperfine and electroweak interaction parameters, parity non-conservation effect in heavy atomic systems. In fact the nuclear-relativistic many-body perturbation theory is based on the combining ab initio perturbation theory formalism for electron subsystem, nuclear relativistic middle-field model for nuclear subsystem and an energy approach for computing radiation transition amplitude and allows to fulfil computing the finite Fermi-systems (5.atomic systems) with taking into account the relativistic, correlation, nuclear, radiative effects. The important feature is the correct accounting for the inter electron correlations, nuclear, Breit and QED radiative corrections. All correlation corrections of the second order and dominated classes of the higher orders diagrams are taken into account.

The results of accurate calculation of the hyperfine structure parameters for the caesium are listed. There are presented the values of the nuclear spin dependent corrections to the PNC ^{133}Cs: 6s-7s amplitude, calculated on the basis of different theoretical methods. The estimated values of a weak charge Q_W for different heavy atoms (5.^{133}Cs, ^{173}Yb and others) are presented and compared with alternative theoretical data

The parity non-conservation (5.PNC) or violation experiments in atomic physics provide an important possibility to deduce information on the Standard Model independent of high-energy physics experiments [1-12]. The recent LEP experiments are fulfilled [1,2], that yield extremely accurate values for Z-boson properties.

In the last two decades a status of the Standard model has been strengthened by different experimental achievements of particle physics. It should be mentioned Higgs boson discovery, measurement of CP violations in the K^-, B^- mesons, evidence of accelerated expansion of the universe, determination of the

fraction of dark energy and dark matter in the universe, etc. From the other side, there are a number of the serious factors which clearly points to some new physics beyond the Standard model despite the desperate lack of direct experimental evidence. One could remind that the density of matter included into the Standard model is approximately 5% of the energy density of the universe; besides, neutrinos in the Standard model are massless, and there are no neutrino oscillations (5.not to mention gravity). As it is known, the Standard model can be divided into three sectors: the calibration sector, the fragrance sector, and the symmetry-breaking sector. While the first two sectors are being actively studied in accelerator experiments (5.LEP, SLD, BELLE, etc.), the sector of spontaneous symmetry breaking is now attracting close attention, as it may give clear hints of existence in New Physics experiments beyond the Standard model. The observation of a static electric dipole moment of a many-electron atom which violates parity, P, and time reversal, T , symmetry, represents a great fundamental interest in a search of these hints. The detailed review of these topics can be found in Refs. [1-91].

Atomic optical and Stark pumping PNC measurements have been fulfilled in a whole number of heavy atoms, namely, in caesium (5.0.35 % accuracy [1]), thallium (5.1.7 %), bismuth (5.2 %), Pb (5.1.2 %) etc. The atomic optical tests of the Standard model provide important constraints on possible extensions of the SM. A recent analysis [2] of parity-violating electron-nucleus scattering measurements combined with atomic PNC measurements placed tight constraints on the weak neutral-current lepton-quark interactions at low energy, improving the lower bound on the scale of relevant new physics to ~ TeV. The precise measurement of the PNC amplitudes in Cs [1] led to an experimental value of the small contribution from the nuclear-spin dependent PNC accurate to 14%. So, form the one side there is very actual necessity of the further development and increasing of the theoretical approaches accuracy and carrying out new atomic optical and Stark pumping PNC experiments.

The different methods have been used in calculation of the hyperfine structure parameters, PNC effect. The most popular multiconfiguration Dirac-Fock (5.MCDF) method for calculating parity and time reversal symmetry violations in many-electron atoms is often, however it application requires some additional

generalizations [3,17,26]. Among other well-known calculation methods, a relativistic many-body perturbation theory (5.RMBPT), namely, the PT with relativistic Hartree-Fock (5.RHF) and Dirac-Fock (5.DF) zeroth approximations, the relativistic all-order method, QED perturbation theory (5.PT) etc should be mentioned (5.e.g.[9-70].

In present chapter we present the application of the consistent theoretical approach, namely, the nuclear-relativistic many-body perturbation theory (5.N-RMBPT), to study the hyperfine and electroweak interaction parameters in the heavy finite Fermi-systems and PNC effect. The N-RMBPT formalism is based on the combining ab initio perturbation theory formalism for electron subsystem, nuclear relativistic middle-field model for nuclear subsystem and an energy approach for computing radiation transition amplitude. It allows to fulfil computing the PNC amplitudes in the finite Fermi-systems (5.atomic systems) [3,10,41,42,49-54,92-101]. The important feature is the correct accounting for the inter electron correlations, nuclear, Breit and QED radiative corrections. All correlation corrections of the second order and dominated classes of the higher orders diagrams are taken into account. The results of calculation of the hyperfine structure parameters, the PNC amplitudes, the nuclear spin dependent corrections to the PNC, a weak charge Q_W for different atomic systems are presented and compared with available data in the literature.

5.2. Relativistic nuclear-RMBPT formalism in theory of heavy finite Fermi-systems

Here we present a brief description of the key moments of our approach **(5.**more details can be found in refs. [3,4,10, 64-98]). The wave electron functions zeroth basis is found from the Dirac equation solution with potential, which includes the self-consistent ab initio potential (5.in the Dirac-Kohn-Sham approximation), electric, polarization potentials of a nucleus. All correlation corrections of the second and high orders of PT (5.electrons screening, particle-hole interaction etc.) are accounted for.

The concrete model for nuclear subsystem is based on the relativistic mean-field model for the ground-state calculation of the nucleus, which was developed

as a renormalizable meson-field theory for nuclear matter and finite nuclei. The realization of nonlinear self-interactions of the scalar meson led to a quantitative description of nuclear ground states. As a self-consistent mean-field model (5.for a comprehensive review see ref. [37,101]), its ansatz is a Lagrangian or Hamiltonian that incorporates the effective, in-medium nucleon-nucleon interaction. As a Kohn-Sham scheme, the relativistic mean-field model can incorporate certain ground-state correlations and yields a ground-state description beyond the literal mean-field picture. As indicated in Refs. [37,38] the strong attractive scalar (5.*S:* -400 MeV) and repulsive vector (5.*V:* +350 MeV) fields provide both the binding mechanism (5.*S* + *V:* -50 MeV) and the strong spin-orbit force (5.*S* – *V:* -750 MeV) of both right sign and magnitude. In our opinion, the most preferable one for the class of problems under consideration is so called NL3-NLC version (5.see details in refs. [3,61,69]), which are among the most successful parameterizations available.

Let us consider the procedure of computing the PNC transition amplitude. The dominative contribution to the PNC amplitude is provided by the spin-independent part of the operator for a weak interaction, which should be added to the atomic Hamiltonian [3]:

$$H = H_{at} + \mu \sum_j H_W(j), \tag{5.1}$$

$$H_W^1 = \frac{G}{2\sqrt{2}} Q_W \gamma_5 \rho(r)., \tag{5.2}$$

Here $G_F = g^2 / 4\sqrt{2} m_W^2$ is the Fermi constant of the weak interaction, γ_5 –is the Dirac matrix, $\rho(5.r)$ is a density of the charge distribution in a nucleus and Q_W is a weak charge of a nucleus, linked with number of neutrons N and protons Z and the Weinberg angle θ_W in the Standard model (5.c.f. [2,5]):

$$Q_W = Z(1 - 4\sin^2 \theta_W) - N \tag{5.3}$$

with accounting for the radiative corrections, equation (5.2) can be rewritten as [1,2]:

$$Q_W = \{Z(1-[4.012 \pm 0.010]\sin^2\theta_W) - N\} \cdot (0.9857 \pm 0.0004)(1 + 0.0078T)$$

$$\sin^2\theta_W = 0.2323 + 0.00365S - 0.00261T) \qquad (5.4)$$

The parameters S, T parameterize the looped corrections in the terms of conservation (5.S) and violation (5.T) of an isospin.

The spin-dependent contribution to the PNC amplitude has a few distinct sources: the nuclear anapole moment (5.(5.that is considered as an electromagnetic characteristics of system, where the PNC takes a place; generally speaking, speech is about the arisen spin structure and the magnetic field distribution is similar to the solenoid field), the *Z*-boson exchange interaction from nucleon axial-vector currents (5.A_nV_e), and the combined action of the hyperfine interaction and spin-independent *Z*-boson exchange from nucleon vector (5.V_nA_e) currents (5.e.g.[3,10,28])

The above-mentioned interactions can be represented by the Hamiltonian

$$H_W^i = \frac{G}{\sqrt{2}} k_i (\alpha \cdot I)\rho(r) \qquad (5.5)$$

where *k*(5.*i*=*a*) is an anapole contribution, k(5.i=2)=k_{Z0} - axial-vector contribution, *k*(5.*i*=*kh*)=k_{Qw} is a contribution due to the combined action of the hyperfine interaction and spin-independent *Z* exchange. It is well known that the contribution into a PNC amplitude, provided by the anapole moment term, significantly dominates.

The estimate of the corresponding matrix elements is in fact reduced to the calculation of the following integrals [10]:

$$< i \mid H_W^1 \mid j >= i\frac{G}{2\sqrt{2}} Q_W \delta_{k_i - k_j} \delta_{m_i m_j} \int_0^\infty dr[F_i(r)G_j(r) - G_i(r)F_j(r)]\rho(r)$$

(5.6)

The reduced matrix element is as follows:

$$< i \| H_W^1 \| j >= i \frac{G}{2\sqrt{2}} Q_W \int_0^\infty dr[F_i(r)G_j(r) - G_i(r)F_j(r)]\rho(r) \qquad (5.7)$$

Further the general expression for the corresponding PNC amplitude for a-b transition is written as follows:

$$< a \mid PNC \mid b >= -\sum_n [\frac{< b \mid e\alpha_\nu A^\nu \mid n >< n \mid H_W^{(1)} \mid a >}{\varepsilon_a - \varepsilon_n} + \frac{< b \mid H_W^{(1)} \mid n >< n \mid e\alpha_\nu A^\nu \mid a >}{\varepsilon_b - \varepsilon_n} \qquad (5.8)$$

The corresponding spin-dependent PNC contribution is:

$$< a \mid PNC \mid b >^{sd} = k_a < a \mid PNC \mid b >^{(a)} + k_2 < a \mid PNC \mid b >^{(2)} + k_{hf} < a \mid PNC \mid b >^{(hf)} , \qquad (5.9)$$

where

$$< a \mid PNC \mid b >^{(hf)} =$$

$$\sum_{\substack{m\neq a \\ n\neq a}} \frac{< a \mid H_W^{(1)} \mid n >< n \mid H_W^{(hf)} \mid m >< m \mid e\alpha_\nu A^\nu \mid b >}{(\varepsilon_a - \varepsilon_m)(\varepsilon_a - \varepsilon_n)} + \sum_{\substack{m\neq a \\ n\neq a}} \frac{< a \mid H_W^{(hf)} \mid n >< n \mid H_W^{(1)} \mid m >< m \mid e\alpha_\nu A^\nu \mid b >}{(\varepsilon_a - \varepsilon_m)(\varepsilon_a - \varepsilon_n)}$$

$$+ \sum_{\substack{m\neq a \\ n\neq b}} \frac{< a \mid H_W^{(1)} \mid m >< m \mid e\alpha_\nu A^\nu \mid n >< n \mid H_W^{(hf)} \mid m >}{(\varepsilon_a - \varepsilon_m)(\varepsilon_b - \varepsilon_n)} + \sum_{\substack{m\neq a \\ n\neq b}} \frac{< a \mid H_W^{(hf)} \mid m >< m \mid e\alpha_\nu A^\nu \mid n >< n \mid H_W^{(hf)} \mid b >}{(\varepsilon_a - \varepsilon_m)(\varepsilon_b - \varepsilon_n)}$$

$$+ \sum_{\substack{m\neq b \\ n\neq b}} \frac{< a \mid e\alpha_\nu A^\nu \mid n >< n \mid H_W^{(1)} \mid m >< m \mid H_W^{(hf)} \mid b >}{(\varepsilon_b - \varepsilon_m)(\varepsilon_b - \varepsilon_n)} + \sum_{\substack{m\neq b \\ n\neq b}} \frac{< a \mid e\alpha_\nu A^\nu \mid n >< n \mid H_W^{(hf)} \mid m >< m \mid H_W^{(1)} \mid b >}{(\varepsilon_b - \varepsilon_m)(\varepsilon_b - \varepsilon_n)}$$

$$- < a \mid H_W^{(hf)} \mid a > \sum_{m\neq a} \frac{< a \mid H_W^{(1)} \mid m >< m \mid e\alpha_\nu A^\nu \mid b >}{(\varepsilon_a - \varepsilon_m)^2} - \sum_{n\neq b} \frac{< a \mid e\alpha_\nu A^\nu \mid n >< n \mid H_W^{(1)} \mid b >}{(\varepsilon_b - \varepsilon_n)^2} < b \mid H_W^{(hf)} \mid b > . \qquad (5.10)$$

Here the following notations are used: $\mid a >= \mid aIF_F M_F >$, $\mid b >= \mid bIF_I M_I >$, I – spin of a nucleus, $F_{I,F}$-is a total momentum of an atom and M – its z component (5.I,F are the initial and final states). It should be noted the expressions for the matrix elements $< a \mid PNC \mid b >^{(a)}$, $< a \mid PNC \mid b >^{(2)}$ are similar to equation (5.10). The full descrip-

tion of the corresponding matrix elements and other details of the general method and PC code are presented in refs. [3,4,10, 64-100].

The fundamentals of the RMBPT formalism are presented previously in details in Refs. [41-50] and here we mention only the key points. The RMBPT formalism includes the optimized Dirac-Kohn-Sham (5.DKS) zeroth approximation and allows to provide an effective taking the relativistic, exchange-correlation, nuclear, radiative effects into account. The relativistic electron wave functions are determined from solution of the relativistic Dirac equation with a general potential. The latter includes ab initio mean-field potential, electric, polarization potentials of a nucleus. There have been considered all correlation corrections of the second order and dominated classes of the higher orders diagrams (5.electrons screening, mass operator iterations etc).

A multielectron system is described by the relativistic Dirac Hamiltonian (5.the atomic units are used) as follows [3,4]:

$$H = \sum_i \{\alpha c p_i - \beta c^2 - Z / r_i\} + \sum_{i>j} \exp(i \mid \omega \mid r_{ij})(1 - \alpha_i \alpha_j)/r_{ij} \tag{5.11}$$

where Z is a charge of nucleus, α_i ,α_j are the Dirac matrices, ω_{ij} is the transition frequency, c – the velocity of light. The interelectron interaction potential second term in (5.3)) takes into account the retarding effect and magnetic interaction in the lowest order on parameter of the fine structure constant α^2 (5.α is the fine structure constant). The mean-field self-consistent potential in the zeroth–order Hamiltonian is as follows:

$$V_{MF} = V^{DKS}(r) = [V^D_{Coul}(r) + V_X(r) + V_C(r \mid b)] \tag{5.12}$$

with the standard Coulomb-like potential $V^D_{Coul}(r)$, is the Kohn-Sham exchange potential $V_x(r)$ [39]:

$$V_X[\rho(r), r] = V_X^{KS}(r) \cdot \{\frac{3}{2} \ln \frac{[\beta + (\beta^2 + 1)^{1/2}]}{\beta(\beta^2 + 1)^{1/2}} - \frac{1}{2}\}, \tag{5.13a}$$

$$\beta = [3\pi^2 \rho(r)]^{1/3} / c \qquad (5.13b)$$

and a correlation functional $V_c(r|b)$, taken in the Lundqvist-Gunnarsson form [4] with ab intio optimization parameter *b* (5.for details, see below and Refs. [42,55-60]).

The approach includes a generalized procedure (5.based on an relativistic energy approach) of generating the optimal basis set of relativistic electron wave functions with performance of the gauge invariance principle. To reach the latter we focus on accurate consideration of the QED PT fourth order (5.a second order of the atomic perturbation theory) Feynman diagrams, whose contribution into imaginary part of radiation width Im δE for the multi-electron ions accounts for multi-body correlation effects.

This value is considered to be representative for the correlation effects, whose minimization is a reasonable criterion in the searching for the optimal one-electron basis of the many-body PT. A minimization of the functional ImδE leads to integral-differential Dirac-Kohn-Sham-like density functional equations. The magnetic inter-electron interaction is accounted for in the lowest order on α^2 (5.α is the fine structure constant) parameter.

The Coulomb-like potential of a nucleus (5.for the spherically symmetric nuclear density $\rho(r|R)$) is determined as follows:

$$V_{nucl}(r|R) = -(1/r)\int_0^r dr' r'^2 \rho(r'|R) + \int_r^\infty dr' r' \rho(r'|R) \qquad (5.14)$$

To take into account the radiation (5.QED) corrections, we used the procedures, described detail in Refs. [41-50,82-87]. A method for calculation of the self-energy part of the Lamb shift is based on an idea by Ivanov-Ivanova et al (5.e.g. [40]), which generalizes the known hydrogen-like method by Mohr [35] and radiation model potential method by Flambaum-Ginges [36] (5.look details in Refs. [3,10,61,69,82-87]). According to Ref. [40], the radiative shift and the relativistic part of energy in an atomic system are, in principle, defined by one and the same physical field. One could suppose that there exists some universal

function that connects the self-energy correction and the relativistic energy. It is worth to note that the low-energy part of the Lamb shift is determined by the following expression:

$$E_H(\Lambda) = \mathrm{Re}\frac{1}{\pi Z}\int_0^\infty d\,\xi\,[E(\xi,0) - E(\xi,\Lambda)], \qquad (5.15a)$$

$$E_H(\xi,\Lambda) = \iint d\,r_1 d\,r_2 \frac{1}{r_{12}} \exp\left[(E_0 - i\xi)^2 - \Lambda^2\right]^{1/2} \Psi^+(r_2)\alpha^\mu G(r_1 r_2)\alpha^\mu \Psi(r_1), \quad (5.15b)$$

(5.here $\Psi(r)$is the Dirac function, an energy parameter $E = i\xi$ is imaginary, G is the complex Green's function) and calculated by means of the complex Green function method in version [91]. The important radiation contributions are given by the standard Uehling-Serber term and the Källen-Sabry and Wichmann-Kroll corrections of higher orders (5.such as $[\alpha\,(Z\alpha)]^n$ (5.n=2,..), $\alpha^2(\alpha Z)$, $\alpha\,(Z\alpha)^n$ (5.n=3) etc; α is the fine structure constant). In order to take into consideration the effect of the vacuum polarization in the first PT order the generalized Uehling-Serber potential is used and modified to account for the high-order radiative corrections according to the procedure [3]. It is written as follows:

$$U(r) = -\frac{2\alpha}{3\pi r}\int_1^\infty dt \exp(-2rt/\alpha Z)\left(1 + 1/2t^2\right)\frac{\sqrt{t^2-1}}{t^2} \equiv -\frac{2\alpha}{3\pi r}C(g), \qquad (5.16)$$

where $g=r/(5.\alpha Z)$. A More correct and consistent approach is presented in Refs. [3,10,61,69,82-87]. Taking into account the nuclear finite size effect modifies the potential (5.16) as follows [3]:

$$U^{FS}(r) = -\frac{2\alpha^2}{3\pi}\int d^3r' \int_1^\infty dt \exp\left(-2t|r-r'|/\alpha Z\right) \times \left(1 + \frac{1}{2t^2}\right)\frac{\sqrt{t^2-1}}{t^2}\frac{\rho(r')}{|r-r'|}, \qquad (5.17)$$

Other details of the general method and PC code are described in Refs. [3,4,10,54-99]. All calculations are performed with using the numeral codes SuperAtom (5.Nucleus) (5.modified versions 93).

5.3. Results and Conclusions

As the first illustration (5.the test), we consider ^{133}Cs and present the results (5.table 1) of calculation of the hyperfine structure (5.hfs) parameters for Cs. In table 1 the experimental (5.A^{Exp}) and our (5.$A^{N\text{-}Qed}$) data for magnetic dipole constant A (5.MHz) for valent states of ^{133}Cs (5.$I=7/2$, $g_i=0.7377208$) are presented. The calculation results within standard (5.A^{RHF}) RHF and RHF with accounting for the second and higher PT corrections, the MCDF approximation and QED formalism are given too (5.from Refs. [3,22-34,63,69]). The following notations are used: A^{RCC} – calculation by relativistic cluster-coupled (5.RCC) method; A^{DF} – DF method; A^{RHF} - RHF method and A^{QED}- the QED calculation; $A^{N\text{-}Qed}$ is the result of this work. The key quantitative factor of physically reasonable agreement between theory and experimental data is connected with the correct accounting for the inter electron correlations, nuclear, Breit and QED radiative corrections.

Table 5.1. The values (5.MHZ) of the hfs constant A for valent states of ^{133}Cs: A^{Exp} - experiment; A^{RHF}, dA^{RHF} - RHF calculation plus the second and higher PT orders contribution [A^{QED} – data]; $A^{N\text{-}Qed}$ – this work

State	A^{MCDF}	A^{RHF}	$A^{RHF}+dA$	A^{Qed}	$A^{N\text{-}Qed}$	A^{Exp}
$6s_{1/2}$	1736.9	1426.81	2291.00	2294.45	2296.78	2298.16 (5.13)
$6p_{1/2}$	209.6	161.09	292.67	292.102	292.118	291.90(5.13)

In table 2 the PNC amplitudes (5.in units of $10^{-11}ie a_B(5.-Q_W)/N$) are listed and calculated on the basis of the different methods (5.without the Breit corrections): DF, RHF, MCDF, MBPT and nuclear-RMBPT results (5.data from refs. [3,22-34,63,69]).

Table 5.2. PNC amplitudes (5.in units of $10^{-11}ie a_B(5.-Q_W)/N$), which are calculated by different methods (without the Breit corrections): DF, RHF, MCDF, MBPT and nuclear-QED PT

Atom Trans.	Spin of Nucl	Nucl. moment (μ_N)	Radius (5.fm) of nucleus	DF	RHF	MCDF	MBPT	N-RMBPT
^{85}Rb 5s-6s	5/2	1.3534	4.246	-0.11	-0.13	-0.13	-0.13	-0.132
^{133}Cs 6s-7s	7/2	2.5826	4.837	-0.74	-0.92 -0.89	-0.90	-0.90 -0.90	-0.903
^{223}Fr 7s-8s	3/2	1.1703	5.640	-13.7	-16.6	-15.7	-15.5 -15.8	-15.54
^{211}Fr 7s-8s	9/2	4.0032	5.539	-12.5	-15.1	-14.3	-	-14.17

In table 3 we present the Breit correction (5.in units of $10^{-11}(5.-Q_W)/N$) to the PNC amplitude, which are calculated by the different methods (5.without the Breit corrections): DF, RHF, MCDF, and nuclear-RMBPT (5.data from Refs. [3,22-34,63,69]). Let us note that the radiative corrections to the PNC amplitude, provided by the vacuum-polarization (5.VP) effect and the self-energy (5.SE) part are as follows: E_{PNC}- ^{133}Cs - VP=0.38%, SE=-0.74%; ^{223}Fr - VP=1.025%, SE=-1.35%.

Table5. 3. The Breit correction (in units of $10^{-11}(-Q_W)/N$) to the PNC amplitude, which are calculated by the different methods (without the Breit corrections): DF, RHF, MCDF, and nuclear-RMBPT results (other data from refs. [25,29,33])

Atom: Transition.	DF	RHF	MCDF	N-QED PT
^{133}Cs 6s-7s	0.0022	0.0018	0.0045	0.0049
^{223}Fr 7s-8s	0.0640	0.0650	**0.1430**	**0.1703**

In table 5.4 we list the nuclear spin dependent corrections to PNC (5.^{133}Cs: 6s-7s) amplitude, calculated by different theoretical methods (5.in units of the $k_{a,2,hf}$ coefficient): MBPT, DF-PT, the shell model, N-RMBPT (5.from Refs. [3,22-34,63,69]).

Table 5.4. The nuclear spin-dependent corrections to the PNC ^{133}Cs: 6s-7s amplitude E_{PNC}, calculated by different methods (5.in units of $k_{a,2,hf}$ coeff.): MBPT, DF-PT, shell model,
N-RMBPT (5.see text)

Correction	MBPT	Shell model	DF	N-RMBPT
K (5.sum)	0.1169	0.1118	0.112	0.1159
k_2- the *Z*-boson exchange interaction from nucleon axial-vector currents (5.A_nV_e)	0.0140	0.0140	0.0111 0.0084	0.0138
k_{hf} - the combined action of the hyperfine interaction and spin-independent *Z* exchange	0.0049	0.0078	0.0071 0.0078	0.0067
k_a –anapole moment	0.0980	0.090	0.0920	0.0954

In table 5.5 we present the estimated values of the weak charge Q_W for different heavy atoms, predicted in different approaches and determined in the Standard model (SM) (from Rrefs. [1-7,22-34,63,69]).

The analysis of results shows that in principle a majority of theoretical approaches provide physically reasonable agreement with the Standard model data, but the important question is how much exact this agreement is. Some re-

ceived data on estimating these constants directly indicate the necessity of new adequate précised experiments.

Table 5.5. The estimated values of the weak charge Q_W and final PNC amplitudes (in units $10^{-11}ie a_B(-Q_W)/N$) for different heavy atoms, predicted in different approaches

Contribution	E_{PNC} Q_W	N-RMBPT	MCDF	MBPT-DF	MCDF QED	RHF+Breit+ Correlation	RCC
^{85}Rb 5s-6s	E_{PNC}	-0.1318	-0.135	-	-	-0.134	-
^{133}Cs 6s-7s	E_{PNC}	-0.8985	-0.935 -0.905	-0.897 -0.904	-0.898 -0.905	-0.898 -0.910 -0.902	- 0.9054 -0.899
^{133}Cs 6s-7s $Q_W^{SM} = -73.19(13)$	Q_W	-72.62	-69.78 -71.09	-72.69 -72.18	-72.65 -72.06	-72.66 -71.70 -72.42	-72.06 -72.58
$^{137}Ba^+$ 6s-5d$_{3/2}$	E_{PNC}	-2.385	-	-2.35	-	-2.34	-2.46
^{173}Yb 6s^2 $^1S_0$-5d6s $^3D_1$ $Q_W^{SM} = -95.44(8)$	E_{PNC} Q_W	-97.07 -92.31	- -	- -	- -	- -	- -
^{205}Tl 6p$_{1/2}$-6p$_{3/2}$	E_{PNC}	26.5114	-26.75	-26.5	-	-	-
^{205}Tl 6p$_{1/2}$-6p$_{3/2}$ $Q_W^{SM} = -116.81(4)$	Q_W	-116.55	-112.4	-116.2 -116:7	-	-	-

The rare-earth elements (5.and corresponding multicharged ions), in particular, ytterbium, are especially interesting as they have very complicated spectra of energy levels with very unusual behavior in relatively weak electric and laser fields. In our opinion, particular attention should be paid to the ^{173}Yb ytterbium atom, where the theoretical PNC values of the EPNC amplitude differ from sim-

ilar values of all considered heavy alkaline atoms by almost two orders of magnitude, which makes this atom particularly important in terms of studying the weak electron-nuclear interaction , the PNC effect, and of course, the Standard model check.

Excessive complexity of the ^{173}Yb calculation, where the correlation effects corrections (including quick “blurring” of the initial state over an infinite set of additional configurations and other effects) is very large, making it difficult to obtain data on the fundamental parameters of Yb. Using the experimental value $\Delta E_1^{PNC}/\beta$ [11]:

$$(8.7\pm1.4)10^{-10}ea_B\ (\Delta E_1^{PNC}/\beta=39\ \text{mV/cm})$$

and the calculated atomic constant value of $99.707\cdot10^{-10}ea_B$ (5.for 173Yb; Z = 70, N = 103) it is not difficult to determine the value of a weak charge Q_W = -92.31, which is different from Q_W (5.the Stanard model)= -95.44. This circumstance imposes unambiguous restrictions on the fundamental values of S, T. It is interesting to note that the estimate of difference [QW (5.theoretical) - QW (5.CM)] ~ 6 indicated in [11] in our opinion, is a little overestimated due to the neglect of the contribution of QED, neutron skin effects etc. Perhaps the increase in the PNC effect at ^{173}Yb can be explained qualitatively and quantitatively in terms of a quantum chaos theory and strong inter-electron correlations (5.e.g.[3,100]).

In any case, it is worth noting the "sensitivity" of PNC experiments to New Physics at energies, which even today are difficult to reach on modern colliders, including the restrictions on the mass of the Z 'boson and the mixing angle in models beyond the Standard model.

The analysis shows that the perspectives of the PNC experiments with Stark pumping of the individual states in the rare-earth atoms (5.and probably more effective multicharged ions of these elements) and simultaneously polarized laser field dressing (5.with a cold-atom fountain or interferometer) may provide comfortable conditions for precise observation of weak effects.

5.4. References

1. Grojean C (5.2007) New approaches to electroweak symmetry breaking. Physics-Uspekhi 50:3-42; Review of Particle Properties (5.1996) Particle Physics Booklet. AIP. July, 1996.
2. Shabalin EP (5.2001) What future for CP- and T-violation studies and CPT-invariance tests? Physics-Uspekhi 171: 951-976.
3. Khetselius OYu (5.2011) Quantum structure of electroweak interaction in heavy finite Fermi-systems. Astroprint, Odessa
4. Glushkov AV 92008) Relativistic Quantum Theory. Quantum, mechanics of atomic Systems. Astroprint, Odessa.
5. Khriplovich IB (5.1991) Parity Nonconservation in Atomic Phenomena. Gordon and Breach, Philadelphia.
6. Grojean C (5.2007) New approaches to electroweak symmetry breaking. Physics-Uspekhi 177: 3-42.
7. Khriplovich IB (5.1997) Discovery of anapole moment. Physics-Uspekhi 167:1214-1216.
8. Auerbach N (5.2008) Search for electric dipole moments in atoms of radioactive nuclei. J Phys G: Nucl Part Phys 35:P014040.
9. Safronova MS, Rupsi P, Jiang D et al (5.2009) New directions in atomic PNC. Nucl Phys A 827: 411-413.
10. Khetselius OYu (5.2008) Hyperfine structure of atomic spectra. Astroprint, Odessa.
11. Tsigutkin K, Dounas-Frazer D, Family A, Stalnaker JE, Yashchuk VV, Budker D (5.2009) Observation of a Large Atomic Parity Violation Effect in Ytterbium. Phys.Rev.Lett. 103:071601.
12. Nagasawa T, Haga A, Nakano M (5.2004) Hyperfine splitting of hydrogenlike atoms based on relativistic mean field theory. Phys Rev C 2004 69:P034322:1-10.
13. Bouchiat MA (5.2007) Linear Stark effect in dressed atoms as a signal to measure a nuclear anapole moment with a cold-atom fountain or interferometer. Phys Rev Lett 98:P043003.

14. Tomaselli M, Kuhl T, Seelig P et al (5.1998) Hyperfine splittings of hydrogenlike ions and the dynamic-correlation model for one-hole nuclei. Phys Rev C 58(5.3)1524-1534.
15. Tomaselli M, Schneider SM, Kankeleit E et al (5.1995) Ground state magnetization of ^{209}Bi in a dynamic-correlation model. Phys Rev C 51(5.6):2989-2997.
16. Labzowsky LN, Johnson WR, Soff G et al (5.1995) Dynamic proton model for the hyperfine structure of H-like ion $^{209}Bi^{+82}$. Phys Rev A 51(5.6):4597-4602.
17. Kozlov_ MG, Porsev SG (5.20010 Parity non-conservation in thallium arXiv:physics/0105090.v1.
18. Porsev SG, Rakhlina YuG, Kozlov MG (5.1995) Non-conservation of spatial parity in atomic ytterbium. JETP Lett 61:449-453.
19. Dzuba VA, Flambaum VV, Sushkov OP (5.1997) Polarizabilities and parity nonconservation in the Cs atom and limits on the deviation from the standard electroweak model. Phys Rev A 56:R4357-4360.
20. Safronova M. S. , Johnson W. R. , Derevianko A (5.1999) Relativistic many-body calculations of energy levels, hyperfine constants, electric-dipole matrix elements, and static polarizabilities for alkali-metal atoms. Phys Rev A 60:P044103.
21. Bennett SC, Roberts JL, Wieman CE (5.1999) Measurement of the dc Stark shift of the 6*S*-7*S* transition in atomic caesium. Phys Rev A 59: 3254-3260.
22. Dzuba VA, Flambaum VV (5.2000) Off-diagonal hyperfine interaction and parity nonconservation in cesium. Phys Rev A 62:P052101.
23. Johnson WR, Bednyakov I, Soff G (5.2001) Vacuum-polarization corrections to the parity-nonconserving 6*s*-7*s* transition amplitude in ^{133}Cs. Phys Rev Lett 87:P233001.
24. Dzuba VA, Harabati C, Johnson WR et al (5.2001) Breit correction to the parity-nonconservation amplitude in cesium. Phys Rev A 63:P044103.
25. Kozlov M.G, Porsev SG, Tupitsyn II (5.2001) High-Accuracy calculation of 6*s*-7*s* parity-nonconserving amplitude in Cs. Phys Rev Lett 86:3260-3263.

26. Johnson WR, Sapistein J, Blundell SA (5.1993) Atomic structure calculations associated with PNC experiments in atomic caesium. Phys Scripta 46:184-192.
27. Vasilyev AA, Savukov IM, Safronova MS et al (5.2002) Measurement of 6*s*-7*p* transition probabilities in atomic Cs and revised value for the weak charge Q_W. Phys Rev A 6:P020101.
28. Johnson WR, Safronova MS, Safronova UI (5.2003) Combined effect of coherent Z exchange and hyperfine interaction in parity-nonconserving interaction. Phys Rev A 67:P062106.
29. Shabaev VM, Tupitsyn II, Pachucki K et al (5.2005) Radiative and correlation effects and parity-nonconserving transition amplitude in heavy alkali-metal atoms. Phys Rev A 72:P062105.
30. Safronova MS, Johnson WR, Safronova UI et al (5.2006) Relativistic many-body theory calculation of the Stark-induced amplitude of the 6p-7p transition in thallium. Phys Rev A 74:P022504.
31. Dzuba VA, Flambaum VV, Safronova MS (5.2006) Breit interaction and parity-nonconservation in many-electron atoms. Phys Rev A 73:P022112.
32. Glushkov AV, Ambrosov SV, Khetselius OYu et al (5.2004) QED calculation of the super heavy elements ions: energy levels, radiative corrections and hfs for different nuclear models. Nucl Phys A: Nucl and Hadr Phys 734:21-28.
33. Kuchiev MYu, Flambaum VV (5.2003) Radiative corrections to parity nonconservation in atoms and test of the standard model. J Phys B 36:R191-222.
34. Johnson WR, Safronova MS, Safronova UI (5.2003) Combined effect of coherent Z exchange and the hyperfine interaction in the atomic parity-non-conserving interaction. Phys Rev A 67:P062106.
35. Mohr PJ (5.1982) Self-energy of the n = 2 states in a strong Coulomb field. Phys Rev A 26:2338.
36. Flambaum VV, Ginges JS (5.2005) Radiative potential and calculations of QED radiative corrections to energy levels and electromagnetic amplitudes in many-electron atoms. Phys Rev A 72:052115.

37. Serot BD, Walecka JD (5.1986) Advances in Nuclear Physics. The Relativistic Nuclear Many Body Problem, vol 16. Plenum Press, New York
38. Burvenich TJ, Evers J, Keitel CH (5.2006) Dynamic nuclear Stark shift in superintense laser fields. Phys. Rev. C. 74:044601.
39. Kohn W, Sham LJ (5.1965) Self-Consistent Equations Including Exchange and Correlation Effects. Phys Rev A 140:1133
40. Ivanov LN, Ivanova EP, Aglitsky EV (5.1988) Modern trends in the spectroscopy of multicharged ions. Phys Rep 166 :315-388.
41. Glushkov AV, Ambrosov SV, Loboda AV, Gurnitskaya EP, Khetselius OY (5.2005) QED calculation of heavy multicharged ions with account for correlation, radiative and nuclear effects. In: Julien J-P, Maruani J, Mayou D, Wilson S, Delgado-Barion G (5.eds) Recent Advances in Theor. Phys. and Chem. Systems. Series: Progress in Theoretical Chemistry and Physics, vol 15. Springer, Dordrecht, pp 285-299.
42. Glushkov AV, Khetselius OYu, Lovett L et al (5.2008) Gauge-invariant QED perturbation theory approach to calculating nuclear electric quadrupole moments, hyperfine structure constants for heavy atoms and ions. Frontiers in Quantum Systems in Chemistry and Physics, vol 18. Berlin, Springer, pp 505-522.
43. Khetselius OYu (5.2008) On sensing nuclei of the lanthanide isotopes by means of laser spectroscopy of hyperfine structure ^{165}Ho, ^{169}Tm. Sensor Electr Microsyst Techn 2:5-9.
44. Khetselius OYu (5.2008) On possibility of sensing nuclei of the rare isotopes by means of laser spectroscopy of hyperfine structure. Sensor Electr Microsyst Techn 3:28-33.
45. Khetselius OYu (5.2009) Relativistic calculating the hyperfine structure parameters for heavy-elements and laser detecting the isotopes and nuclear reaction products. Phys Scripta T 135:P014023.
46. Khetselius OYu (5.2009) On sensing nuclei of the ^{207}Bi &^{207}Pb isotopes by means of laser spectroscopy of hyperfine. Sensor Electr and Microsyst Techn 2:26-29.

47. Khetselius OYu (5.2009) Relativistic perturbation theory calculation of the hyperfine structure parameters for some heavy-element isotopes. Int J of Quantum Chemistry 109:3330-3335.
48. Khetselius OYu (5.2009) Relativistic calculation of the hyperfine structure parameters for heavy elements and laser detection of the heavy isotopes. Phys Scripta 135:014023.
49. Glushkov AV (5.2006) Relativistic and Correlation Effects in Spectra of Atomic Systems. Astroprint, Odessa
50. Khetselius OYu (5.2012) Relativistic Energy Approach to Cooperative Electron-γ-Nuclear Processes: NEET Effect. In: Nishikawa K, Maruani J, Brändas E, Delgado-Barrio G, Piecuch P (5.eds) Quantum Systems in Chemistry and Physics: Progress in Methods and Applications. Series: Progress in Theoretical Chemistry and Physics, vol 26. Springer, Dordrecht, pp 217-229.
51. Glushkov AV, Rusov VD, Ambrosov SV, Loboda AV (5.2003) Resonance states of compound super-heavy nucleus and EPPP in heavy nucleus collisions. In: Fazio G, Hanappe F (5.eds) New Projects and New Lines of Research in Nuclear Physics. World Scientific, Singapore, 126-132.
52. Glushkov AV (5.2005) Energy approach to resonance states of compound superheavy nucleus and EPPP in heavy nuclei collisions. In: Grzonka D, Czyzykiewicz R, Oelert W et al (5.eds) Low Energy Antiproton Physics. AIP Conf Proc, New York, 796:206-210.
53. Glushkov AV (5.2012) Spectroscopy of cooperative muon-gamma-nuclear processes: Energy and spectral parameters. J Phys: Conf Ser 397:012011.
54. Malinovskaya SV, Glushkov AV, Dubrovskaya YV, Vitavetskaya LA (5.2006) Quantum calculation of cooperative muon-nuclear processes: Discharge of metastable nuclei during negative muon capture. In: Julien J-P, Maruani J, Mayou D, Wilson S, Delgado-Barion G (5.eds) Recent Advances in the Theory of Chemical and Physical Systems. Series: Progress in Theoretical Chemistry and Physics, vol 15. Springer, Dordrecht, pp 301–307
55. Glushkov AV, Khetselius OYu, Gurnitskaya EP, Loboda AV, Florko TA,

Sukharev DE, Lovett L (5.2008) Gauge-Invariant QED Perturbation Theory Approach to Calculating Nuclear Electric Quadrupole Moments, Hyperfine Structure Constants for Heavy Atoms and Ions. In: Wilson S, Grout PJ, Maruani J, Delgado-Barrio G, Piecuch P (5.eds) Frontiers in Quantum Systems in Chemistry and Physics. Series: Progress in Theoretical Chemistry and Physics, vol 18. Springer, Dordrecht), pp 507-524.

56. Glushkov AV, Ivanov LN (5.1992) Radiation decay of atomic states: atomic residue polarization and gauge noninvariant contributions. Phys Lett A 170:33-36.
57. Glushkov AV, Ivanov LN., Ivanova EP (5.1986) Radiation decay of atomic states. Generalized energy approach. In: Autoionization Phenomena in Atoms. Moscow State Univ., Moscow, p 58
58. Ivanova E.P, Glushkov AV (5.1986) Theoretical investigation of spectra of multicharged ions of F-like and Ne-like isoelectronic sequences. J Quant Spectr Rad Transfer 36 :127-145.
59. Khetselius OYu (5.2015) Optimized Perturbation Theory for Calculating the Hyperfine Line Shift and Broadening of Heavy Atoms in a Buffer Gas. In: Nascimento M, Maruani J, Brändas E, Delgado-Barrio G (5.eds) Frontiers in Quantum Methods and Applications in Chemistry and Physics. Series: Progress in Theoretical Chemistry and Physics, vol. 29. Springer, Cham, pp. 55-76.
60. Khetselius OYu, Zaichko PA, Smirnov AV, Buyadzhi VV, Ternovsky VB, Florko TA, Mansarliysky VF (5.2017) Relativistic Many-Body Perturbation Theory Calculations of the Hyperfine Structure and Oscillator Strength Parameters for Some Heavy Element Atoms and Ions. In: Tadjer A, Pavlov R, Maruani J, Brändas E, Delgado-Barrio G (5.eds) Quantum Systems in Physics, Chemistry, and Biology. Series: Progress in Theoretical Chemistry and Physics, vol 30. Springer, Cham, pp 271-281.
61. Khetselius OYu, Lopatkin YuM, Dubrovskaya YuV, Svinarenko AA (5.2010) Sensing hyperfine-structure, electroweak interaction and parity non-conservation effect in heavy atoms and nuclei: New nuclear-QED approach. Sensor Electr. And Microsyst. Techn. 7(5.2):11-19.
62. Khetselius OYu (5.2009) Atomic parity non-conservation effect in heavy

atoms and observing P and PT violation using NMR shift in a laser beam: To precise theory. J Phys: Conf Ser 194:022009.

63. Khetselius OYu (5.2010) Relativistic hyperfine structure spectral lines and atomic parity nonconservation effect in heavy atomic systems within QED theory. AIP Conf Proc 1290:29-33.
64. Glushkov AV (5.1992) Oscillator strengths of Cs and Rb-like ions. Journal of Appl Spectroscopy 56(5.1):5-9.
65. Glushkov AV (5.1990) Relativistic polarization potential of a many-electron atom. Sov Phys Journal 33(5.1):1-4.
66. Khetselius Oyu, Zaichko PA, Smirnov AV, Buyadzhi VV, Ternovsky VB, Florko TA, Mansarliysky VF (5.2017) Relativistic Many-Body Perturbation Theory Calculations of the Hyperfine Structure and Oscillator Strength Parameters for Some Heavy Element Atoms and Ions. In: Tadjer A, Pavlov R, Maruani J, Brändas E, Delgado-Barrio G (5.eds) Quantum Systems in Physics, Chemistry, and Biology. Advances in Concepts and Applications. Series: Progress in Theoretical Chemistry and Physics, vol 30. Springer, Cham, pp 271-281.
67. Khetselius OYu, Glushkov AV, Dubrovskaya YuV, Chernyakova YuG, Ignatenko AV, Serga IN, Vitavetskaya LA (5.2018) Relativistic quantum chemistry and spectroscopy of exotic atomic systems with accounting for strong interaction effects. In: Wang YA, Thachuk M, Krems R, Maruani J (5.eds) Concepts, Methods and Applications of Quantum Systems in Chemistry and Physics. Series: Progress in Theoretical Chemistry and Physics, vol 31. Springer, Cham, pp 71-91.
68. Dubrovskaya YuV, Khetselius OYu, Vitavetskaya LA, Ternovsky VB, Serga IN (5.2019) Quantum Chemistry and Spectroscopy of Pionic Atomic Systems with Accounting for Relativistic, Radiative, and Strong Interaction Effects. Adv Quantum Chem. Elsevier. 78:193-222. https://doi.org/10.1016/bs.aiq.2018.06.003.
69. Khetselius O Yu, Glushkov A V, Gurskaya M Yu, Kuznetsova A A, Dubrovskaya Yu V, Serga I N and Vitavetskaya L A (5.2017) Computational modelling parity nonconservation and electroweak interaction ef-

fects in heavy atomic systems within the nuclear-relativistic many-body perturbation theory. J. Phys.: Conf. Ser. 905:012029

70. Glushkov AV, Khetselius OYu, Svinarenko AA, Buyadzhi VV 92015) Spectroscopy of autoionization states of heavy atoms and multiply charged ions. TEC, Odessa.
71. Glushkov AV, Khetselius OYu, Svinarenko AA, Buyadzhi VV (5.2015) Methods of computational mathematics and mathematical physics. P.1. TES, Odessa.
72. Glushkov AV, Malinovskaya SV, Filatov VV (5.1989) S-Matrix formalism calculation of atomic transition probabilities with inclusion of polarization effects. Sov Phys Journal 32(5.12):1010-1014.
73. Glushkov AV, Butenko YuV, Serbov NG, Ambrosov SV, Orlova VE, Orlov SV, Balan AK, Dormostuchenko GM (5.1996) Calculation and extrapolation of oscillator strengths in Rb-like, multiply charged ions. Russian Phys Journ 39(5.1):81-83.
74. Glushkov AV (5.2012) Advanced Relativistic Energy Approach to Radiative Decay Processes in Multielectron Atoms and Multicharged Ions. In: Nishikawa K, Maruani J, Brandas E, Delgado-Barrio G, Piecuch P (5.eds) Quantum Systems in Chemistry and Physics: Progress in Methods and Applications. Series: Progress in Theoretical Chemistry and Physics, vol 26. Springer, Dordrecht, pp 231-252.
75. Glushkov AV (5.2013) Operator Perturbation Theory for Atomic Systems in a Strong DC Electric Field. In: Hotokka M, Brändas E, Maruani J, Delgado-Barrio G (5.eds) Advances in Quantum Methods and Applications in Chemistry, Physics, and Biology. Series: Progress in Theoretical Chemistry and Physics, vol 27 Springer, Cham, pp 161-177.
76. Glushkov AV, Malinovskaya SV, Loboda AV, Shpinareva IM, Gurnitskaya EP, Korchevsky DA (5.2005) Diagnostics of the collisionally pumped plasma and search of the optimal plasma parameters of x-ray lasing: Calculation of electron-collision strengths and rate coefficients for Ne-like plasma. J Phys: Conf Ser 11:188-198.
77. Glushkov AV, Malinovskaya SV, Chernyakova YuG, Svinarenko AA (5.2004) Cooperative Laser-Electron-Nuclear Processes: QED Calcula-

tion of Electron Satellites Spectra for Multi-Charged Ion in Laser Field. Int Journ Quant Chem 99(5.5):889-893.

78. Glushkov AV, Ambrosov SV, Ignatenko AV, Korchevsky DA (5.2004) DC Strong Field Stark Effect for Non-hydrogenic Atoms: New Consistent Quantum Mechanical Approach. Int Journ Quant Chem 99(5.5): 936-939.
79. Glushkov AV, Malinovskaya SV, Loboda AV, Shpinareva IM, Prepelitsa GP (5.2006) Consistent quantum approach to new laser-electron-nuclear effects in diatomic molecules. J Phys: Conf 35:420-424.
80. Malinovskaya SV, Dubrovskaya YuV, Zelentzova TN 92004) The atomic chemical environment effect on the β decay probabilities: Relativistic calculation. Herald of Kiev Nat Univ. Series: Phys Math 4:427-432.
81. Glushkov AV (5.1994) Calculation of parameters of the interaction potential between excited alkali atoms and mercury atoms-the Cs-, Fr-Hg interaction. Opt. and Spectr 77(5.1):5-10.
82. Glushkov AV, Gurskaya MYu, Ignatenko V, Smirnov AV, ISerga IN, Svinarenko AA and Ternovsky EV (5.2017) Computational code in atomic and nuclear quantum optics: Advanced computing multiphoton resonance parameters for atoms in a strong laser field. J Phys: Conf Ser 905:P012004.
83. Svinarenko AA, Glushkov AV, Khetselius OYu, Ternovsky VB, Dubrovskaya YuV, Kuznetsova AA, Buyadzhi VV (5.2017) Theoretical Spectroscopy of Rare-Earth Elements: Spectra and Autoionization Resonance. In: Jose EA (5.ed) Rare Earth Element. InTech, Orjuela, pp 83-104. https://doi.org/10.5772/intechopen.69314.
84. Glushkov AV, Khetselius OYu, Svinarenko AA, Buyadzhi VV, Ternovsky VB, Kuznetsova AA, Bashkarev PG (5.2017) Relativistic Perturbation Theory Formalism to Computing Spectra and Radiation Characteristics: Application to Heavy Element. In: Dimo I (5.ed) Recent Studies in Perturbation Theory. InTech, Uzunov, pp 131-150. https://doi.org/: 10.5772/intechopen.69102.
85. Glushkov AV, Khetselius OYu, Gurnitskaya EP, Loboda AV, Florko TA, Sukharev DE, Lovett L (5.2008) Gauge-Invariant QED Perturbation Theory Approach to Calculating Nuclear Electric Quadrupole Moments, Hy-

perfine Structure Constants for Heavy Atoms and Ions. In: Wilson S, Grout PJ, Maruani J, Delgado-Barrio G, Piecuch P (5.eds) Frontiers in Quantum Systems in Chemistry and Physics. Series: Progress in Theoretical Chemistry and Physics, vol 18. Springer, Dordrecht), pp 507-524.

86. Khetselius OYu, Glushkov AV, Dubrovskaya YuV, Chernyakova YuG, Ignatenko AV, Serga IN, Vitavetskay LA (5.2018) Relativistic quantum chemistry and spectroscopy of exotic atomic systems with accounting for strong interaction effects. In: Wang YA, Thachuk M, Krems R, Maruani J (5.eds) Concepts, Methods and Applications of Quantum Systems in Chemistry and Physics. Series: Progress in Theoretical Chemistry and Physics, vol 31. Springer, Cham, pp 71-91
87. Khetselius OYu (5.2012) Quantum Geometry: New approach to quantization of quasistationary states of Dirac equation for superheavy ion and calculating hyperfine structure parameters. Proc. Intern. Geom. Center 5(5.3-4):39-45
88. Glushkov AV, Rusov VD, Ambrosov SV, Loboda AV (5.2003) Resonance states of compound super-heavy nucleus and EPPP in heavy nucleus collisions. In: Fazio G, Hanappe F (5.eds) New Projects and New Lines of Research in Nuclear Physics. World Scientific, Singapore, 126-132.
89. Glushkov AV, Khetselius OYu, Svinarenko AA (5.2013) Theoretical spectroscopy of autoionization resonances in spectra of lanthanide atoms. Phys Scr T153:014029.
90. Malinovskaya SV, Glushkov AV, Khetselius OYu, Svinarenko AA, Mischenko EV, Florko TA(5.2009) Optimized perturbation theory scheme for calculating the interatomic potentials and hyperfine lines shift for heavy atoms in the buffer inert gas. Int Journ Quant Chem 109:3325-3329
91. Glushkov AV, Malinovskaya SV, Khetselius OYu, Loboda AV, Sukharev DE, Lovett L (5.2009) Green's function method in quantum chemistry: New numerical algorithm for the Dirac equation with complex energy and Fermi-model nuclear potential. Int Journ Quant Chem 109:1717-1727.
92. Glushkov AV, Lovett L, Khetselius OYu, Gurnitskaya EP, Dubrovskaya YuV, Loboda AV (5.2009) Generalized multiconfiguration model of de-

cay of multipole giant resonances applied to analysis of reaction (5.μ-n) on the nucleus ^{40}Ca. Int. Journ. of Modern Phys. A 24(5.2-3):611-615.

93. Glushkov AV, Khetselius OYu, Svinarenko AA (5.2012) Relativistic theory of cooperative muon-γ -nuclear processes: Negative muon capture and metastable nucleus discharge. In: Hoggan P, Brändas E, Maruani J, Delgado-Barrio G, Piecuch P (5.eds) Advances in the Theory of Quantum Systems in Chemistry and Physics. Series: Progress in Theoretical Chemistry and Physics, vol 22. Springer, Dordrecht, pp 51-68.
94. Glushkov A, Khetselius O, Lovett L (5.2009) Electron-β-nuclear spectroscopy of atoms and molecules and chemical bond effect on the β-decay parameters. In: Piecuch P, Maruani J, Delgado-Barrio G, Wilson S (5.eds) Advances in the Theory of Atomic and Molecular Systems Dynamics, Spectroscopy, Clusters, and Nanostructures. Series: Progress in Theor. Chem. and Phys., vol 20. Springer, Dordrecht, pp 125-152.
95. Glushkov AV, Khetselius OYu, Lopatkin YM, Florko TA, Kovalenko OA, Mansarliysky VF (5.2014) Collisional shift of hyperfine line for rubidium in an atmosphere of the buffer inert gas. J of Phys: Conf Ser 548:012026
96. Malinovskaya SV, Dubrovskaya YuV, Vitavetskaya LA (5.2005) Advanced Quantum Mechanical Calculation of the Beta Decay Probabilities. Energy approach to resonance states of compound superheavy nucleus and EPPP in heavy nuclei collisions. In: Low Energy Antiproton Physics; Grzonka, D., Czyzykiewicz, R., Oelert,W., Rozek, T., Winter, P., Eds.; AIP: New York, AIP Conf. Proc. 796:201-205
97. Glushkov AV, Gurskaya M Yu, Ignatenko AV, Smirnov AV, Serga IN, Svinarenko AA, Ternovsky EV (5.2017) Computational code in atomic and nuclear quantum optics: Advanced computing multiphoton resonance parameters for atoms in a strong laser field. J. Phys: Conf. Ser. 905(5.1): 012004.
98. Dubrovskaya YuV, Khetselius OYu, Vitavetskaya LA, Ternovsky VB, Serga IN (5.2019) Quantum Chemistry and Spectroscopy of Pionic Atomic Systems With Accounting for Relativistic, Radiative, and Strong Interaction Effects. Adv Quantum Chem, vol 78. Elsevier, pp 193-222.

https://doi.org/10.1016/bs.aiq.2018.06.003.
99. Glushkov AV, Khetselius OYu, Kruglyak YuA, Ternovsky VB (5.2014) Calculational Methods in Quantum Geometry and Chaos theory. P.3. OSENU(5.TEC), Odessa
100. Glushkov AV (5.2012) Methods of a Chaos Theory. Astroprint, Odessa
101. Furnstahl R J (5.2004) Next generation relativistic models. In: G A Lalazissis, P Ring P, Vretenar D (5.eds) Extended Density Functionals in Nuclear StructurePhysics, vol 641. Springer, Berlin, pp 1-30

CHAPTER 6. GAUGE-INVARIANT QED PERTURBATION THEORY APPROACH TO CALCULATING NUCLEAR ELECTRIC QUADRUPOLE MOMENTS, HYPERFINE STRUCTURE CONSTANTS FOR HEAVY ATOMS AND IONS: SUPERATOM PACKAGE

6.1 Introduction

Relativistic calculation of the spectra hyperfine structure parameters for heavy atoms and multicharged ions with account of relativistic, correlation, nuclear, QED effects is carried out (6.the Superatom package) [11-18]. Our calculation scheme is based on gauge-invariant QED perturbation theory with using the optimized one-quasiparticle representation at first in the theory of the hyperfine structure for relativistic systems [12,14,16]. It is carried out calculating the energies and constants of the hyperfine structure, deriviatives of the one-electron characteristics on nuclear radius, nuclear electric quadrupole, magnetic dipole moments Q for atom of hydrogen ^{1}H (6.test calculation), superheavy H-like ion with nuclear charge Z=170, Li-like multicharged ions with Z=20-100, neutral atoms of ^{235}U, ^{201}Hg and ^{227}Ra are defined.

In last years a studying the spectra of heavy and superheavy elements atoms and ions is of a great interest for further development as atomic and nuclear theories (6.c.f.[1-12]). Theoretical methods used to calculate the spectroscopic characteristics of heavy and superheavy ions may be divided into three main groups: a) the multi-configuration Hartree-Fock method, in which relativistic effects are taken into account in the Pauli approximation, gives a rather rough approximation, which makes it possible to get only a qualitative idea on the spectra of heavy ions. b) The multi-configuration Dirac-Fock (6.MCDF) approximation (6.the Desclaux program, Dirac package) [1-6,22] is, within the last few years, the most reliable version of calculation for multielectron systems with a large nuclear charge; in these calculations one- and two-particle relativistic effects are taken into account practically precisely. The calculation program of Desclaux is compiled with proper account of the finiteness of the nucleus size; however, a detailed description of the method of their investigation of the role of

the nucleus size is lacking. In the region of small Z (6.Z is a charge of the nucleus) the calculation error in the MCDF approximation is connected mainly with incomplete inclusion of the correlation and exchange effects which are only weakly dependent on Z; c) In the study of lower states for ions with $Z \leq 40$ an expansion into double series of the PT on the parameters 1/Z, αZ (6.α is the fine structure constant) turned out to be quite useful. It permits evaluation of relative contributions of the different expansion terms: non-relativistic, relativistic, QED contributions as the functions of Z. Nevertheless, the serious problems in calculation of the heavy elements spectra are connected with developing new, high exact methods of account for the QED effects, in particular, the Lamb shift (6.LS), self-energy (6.SE) part of the Lamb shift, vacuum polarization (6.VP) contribution, correction on the nuclear finite size for superheavy elements and its account for different spectral properties of these systems, including calculating the energies and constants of the hyperfine structure, deriviatives of the one-electron characteristics on nuclear radius, nuclear electric quadrupole, magnetic dipole moments etc (6.c.f.[1-22]).

In present paper a new, highly exact, ab initio approach to relativistic calculation of the spectra for multi-electron superheavy ions with an account of relativistic, correlation, nuclear, radiative effects is presented. The method is based on the quantum electrodynamical (6.QED) perturbation theory (6.PT). Relativistic calculation of the spectra hyperfine structure parameters for heavy atoms and multicharged ions with account of relativistic, correlation, nuclear, QED effects is carried out (6.the Superatom [11-18] and Dirac packages (6.DP) [22] are used; the DP using in a progress). Our calculation scheme is based on gauge-invariant QED perturbation theory and and generelized relativistic dynamical effective field nuclear model with using the optimized one-quasiparticle representation at first in the theory of the hyperfine structure for relativistic systems [11-16]. The wave function zeroth basis is found from the Dirac equation with potential, which includes the core ab initio potential, the electric and polarization potentials of a nucleus (6.the gaussian form of charge distribution in the nucleus is considered) [12-16]. The correlation corrections of the high orders are taken into account within the Green functions method (6.with the use of the Feynman diagram's technique). There have taken into account all correlation corrections of the second order and dominated classes of the higher orders diagrams

(6.electrons screening, particle-hole interaction, mass operator iterations) [11-18]. The magnetic inter-electron interaction is accounted in the lowest (6.on α^2 parameter), the LS polarization part - in the Uehling-Serber approximation, self-energy part of the LS is accounted effectively within the Ivanov-Ivanova non-perturbative procedure [11]. Generelized relativistic dynamical effective field nuclear model is presented in [18] (6.see also refs.[5,6,16]). The energies and constants of the hyperfine structure, deriviatives of the one-electron characteristics on nuclear radius, nuclear electric quadrupole, magnetic dipole moments *Q* for atom of hydrogen ^{1}H (6.test calculation), superheavy H-like ion with nuclear charge Z=170, Li-like multicharged ions with Z=20-100, neutral atoms of ^{235}U, ^{201}Hg and ^{227}Ra are calculated.

6.2. QED perturbation theory method for calculation of heavy and superheavy ions

Let us describe the key moments of our approach to relativistic calculation of the spectra for multi-electron superheavy ions with an account of relativistic, correlation, nuclear, radiative effects **(6.**more details can br found in ref.[11-18]).

One-particle wave functions are found from solution of the relativistic Dirac equation, which can be written in the central field in a two-component form:

$$\frac{\partial F}{\partial r} + (1+\chi)\frac{F}{r} - (\varepsilon + m - v)G = 0$$
$$\frac{\partial G}{\partial r} + (1-\chi)\frac{G}{r} + (\varepsilon - m - v)F = 0 \qquad (6.1)$$

Here we put the fine structure constant α=1 . The moment number

$$\chi = \begin{cases} -(1+1), & j > 1 \\ 1, & j < 1 \end{cases} \qquad (6.2)$$

At large χ the radial functions F and G vary rapidly at the origin of co-ordinates:

$$F(r), G(r) \approx r^{\gamma-1}$$
$$\gamma = \sqrt{\chi^2 - \alpha^2 z^2} \qquad (6.3)$$

This involves difficulties in numerical integration of the equations in the region $r \to 0$. To prevent the integration step becoming too small it is convenient to turn to new functions isolating the main power dependence: $f = Fr^{1-|\chi|}$, $g = Gr^{1-|\chi|}$. The Dirac equation for F and G components are transformed as:

$$f' = -(\chi + |\chi|) f/r - \alpha Z V g - (\alpha Z E_{n\chi} + 2/\alpha Z) g$$
$$g' == (\chi - |\chi|) g/r - \alpha Z V f + \alpha Z E_{n\chi} f \qquad (6.4)$$

Here the Coulomb units (6.C.u.) are used; 1 C.u. of length = 1 a.u.Z; 1 C.u. of energy = 1 a.u. Z^2. In Coulomb units the atomic characteristics vary weakly with Z. $E_{n\chi}$ is one-electron energy without the rest energy, the system of equations (6.4) has two fundamental, solutions. We are interested in the solution regular at $r \to 0$. The boundary values of the correct solution are found by the first term s of the expansion into the Taylor series:

$$g = (V(0) - E_{n\chi}) r\alpha Z/(2\chi + 1); \quad f = 1 \text{ at } \chi < 0$$

$$f = (V(0) - E_{n\chi} - 2/\alpha^2 Z^2)\alpha Z; \quad g = 1 \text{ at } \chi > 0 \qquad (6.5)$$

The condition $f, g \to 0$ at $r \to \infty$ determines the quantified energies of the state $E_{n\chi}$. At correctly determined energy $E_{n\chi}$ of the asymptotic f and g at $r \to \infty$ are:

$$f, g \sim \exp(-r/n^*) \qquad (6.6)$$

where $n^* = \sqrt{1/2|E_{n\chi}|}$ is the effective main quantum number. The equations (6.4) were solved by the Runge-Kutter method. The initial integration point

$r_0 = R/10^6$, where R is the nucleus radius, the end of the integration interval is determined as $r_k \approx 30n^*$.

Earlier we calculated some characteristics of hydrogen-like ions with the nucleus in the form of a uniformly charged sphere; analogous calculations by means of an improved model were also made; Here the smooth Gaussian function of the charge distribution in the nucleus is used. Using the smooth distribution function (6.instead of the discontinuous one) simplifies the calculation procedure and permits flexible simulation of the real distribution of the charge in the nucleus. As in ref. [12] we set the charge distribution in the nucleus $\rho(r)$ by the Gaussian function. With regard to normalization we have:

$$\rho(r|R) = \left(4\gamma^{3/2}/\sqrt{\pi}\right)\exp\left(-\gamma r^2\right) \qquad (6.7)$$

$$\int_0^\infty drr^2\rho(r|R) = 1; \quad \int_0^\infty drr^3\rho(r|R) = R$$

were $\gamma = 4/\pi R^2$, R is the effective nucleus radius. The following simple dependence of *R* on *Z* assumed:

$$R = 1.60\times10^{-13} z^{1/3}\ (cm) \qquad (6.8)$$

Such definition of R is rather conventional. We assume it as some zeroth approximation. Further the derivatives of various characteristics on R are calculated. They describe the interaction of the nucleus with outer electron; this permits recalculation of results, when R varies within reasonable limits. The Coulomb potential for the spherically symmetric density $\rho(r|R)$ is:

$$V_{nucl}(r|R) = -((1/r)\int_0^r dr'r'^2\rho\left(r'\middle|R\right) + \int_r^\infty dr'r'\rho\left(r'\middle|R\right) \qquad (6.9)$$

It is determined by the following system of differential equations:

$$V'nucl(r,R) = \left(1/r^2\right)\int_0^r dr'r'^2\rho\left(r',R\right) \equiv \left(1/r^2\right)y(r,R)$$

$$y'(r,R) = r^2 \rho(r,R) \qquad (6.10)$$

$$\rho'(r,R) = -8\gamma^{5/2}\, r/\sqrt{\pi}\, \exp\left(-\gamma r^2\right) = -2\gamma r \rho(r,R) = -\frac{8r}{\pi r^2}\rho(r,R)$$

with the boundary conditions:

$$V_{nucl}(0,R) = -4/(\pi r)$$

$$y(0,R) = 0\,,$$

$$\rho(0,R) = 4\gamma^{3/2}/\sqrt{\pi} = 32/R^3 \qquad (6.11)$$

Consider the Dirac-Fock type equations for a three-electron system $1s^2 nlj$. Formally they fall into one-electron Dirac equations for the orbitals $1s$ 1s and nlj with the potential:

$$V(r) = 2V(r|1s) + V(r|nlj) + V_{ex}(r) + V(r|R) \qquad (6.12)$$

$V(r|R)$ includes the electrical and the polarization potentials of the nucleus; the components of the Hartree potential:

$$V(r|i) = \frac{1}{Z}\int d\vec{r}\,' \rho(r|i)/|\vec{r} - \vec{r}\,'|$$

(6.13)

$\rho(r|i)$ is the distribution of the electron density in the state | i >, V_{ex} is the exchange inter-electron interaction. The main exchange effect will be taken into account if in the equation for the $1s$ orbital we assume

$$V(r) = V(r|1s) + V(r|nlj) \qquad (6.14)$$

and in the equation for the nlj orbital

$$V(r) = 2V(r|1s) \tag{6.15}$$

The rest of the exchange and correlation effects will be taken into account in the first two orders of the PT by the total inter-electron interaction [13-17].

The used expression for $\rho(r|1s)$ coincides with the precise one for a one-electron relativistic atom with a point nucleus. The finiteness of the nucleus and the presence of the second 1*s* electron are included effectively into the energy E_{1s}. Actually, for determination of the properties of the outer *nlj* electron one iteration is sufficient. Refinement resulting from second iteration (6.by evaluations) does not exceed correlation corrections of the higher orders omitted in the present calculation. The relativistic potential of core (6.the "screening" potential) $2V^{(1)}(r|1s) = V_{scr}$ has correct asymptotic at zero and in the infinity; at $\alpha \to 0$ it changes to an appropriate potential constructed on the basis of non-relativistic hydrogen-like functions.

Procedure for an account of the radiative QED corrections is in details given in the refs. [12,16,17]. Rergartding the vacuum polariation effect let us note that this effect is usually taken into account in the first PT theory order by means of the Uehling potential. This potential is usually written as follows (6.c.f.[1,11]):

$$U(r) = -\frac{2\alpha}{3\pi r}\int_1^\infty dt\,\exp(-2rt/\alpha Z)\left(1+1/2t^2\right)\frac{\sqrt{t^2-1}}{t^2} \equiv -\frac{2\alpha}{3\pi r}C(g), \tag{6.16}$$

where $g = \frac{r}{\alpha Z}$. In our calculation we usually use more exact approach. The Uehling potential, determined as a quadrature (6.16) may be approximated with high precision by a simple analytical function. The use of new approximation of the Uehling potential permits one to decrease the calculation errors for this term down to 0.5 – 1%. Besides, using such a simple analytical function form for approximating the Uehling potential allows its easy inclusion into the general system of differential equations. This system includes also the Dirac equations and the equations for matrix elements. A method for calculation of the self-energy part of the Lamb shift is based on an idea by Ivanov-Ivanova (6.c.f.[12,17]). In an atomic system the radiative shift and the relativistic part of

the energy are, in. principle, determined by one and the same physical field. It may be supposed that there exists some universal function that connects the self -energy correction and the relativistic energy. The self-energy correction for the states of a hydrogen-like ion was presented by Mohr [1] as:

$$E_{SE}(H|Z,nlj) = 0.027148\,\frac{Z^4}{n^3}\,F(H|Z,nlj) \qquad (6.17)$$

The values of F are given at $Z = 10-110,\ nlj = 1s,2s,2p_{1/2},2p_{3/2}$. These results are modified here for the states $1s^2\ nlj$ of Li-like ions. It is supposed that for any ion with *nlj* electron over the core of closed shells the sought value may be presented in the form:

$$E_{SE}(Z,nlj) = 0.027148\,\frac{\xi^4}{n^3}\,f(\xi,nlj)\left(cm^{-1}\right) \qquad (6.18)$$

The parameter $\xi = (E_R)^{1/4},\ E_R$ is the relativistic part of the bounding energy of the outer electron; the universal function $f(\xi,nlj)$ does not depend on the composition of the closed shells and the actual potential of the nucleus. The procedure of generalization for a case of Li-like ions with the finite nucleus consists of the following steps [17]:

1). Calculation of the values E_R and ξ for the states *nlj* of H-like ions with the point nucleus (6.in accordance with the Zommerfeld formula);

2). Construction of an approximating function $f(\xi,nlj)$ by the found reference *Z* and the appropriate $F(H|Z,nlj)$ [1,11];

3). Calculation of E_R and ξ for the states *nlj* of *Li*-like ions with the finite nucleus; 4). Calculation of E_{SE} for the sought states by the formula (6.18). The energies of the states of Li-like ions were calculated twice: with a conventional constant of the fine structure $\alpha = 1/137$ and with $\tilde{\alpha} = \alpha/1000$. The results of latter calculations were considered as non-relativistic. This permitted isolation of E_R and ξ. A detailed evaluation of their accuracy may be made only after a complete calculation of $E^n_{SE}(Li\,Z,nlj)$. It may be stated that the above extrapolation method is more justified than using the widely spread expansions by the parameter αZ.

Energies of the quadruple ($6.W_q$) and magnetic dipole ($6.W_\mu$) interactions, which define a hyperfine structure, are calculated as follows [11,20]:

$$W_q=[\Delta+C(C+1)]B,$$

$$W_\mu=0{,}5\,AC,$$

$$\Delta=-(4/3)(4\chi-1)(I+1)/[i(I-1)(2I-1)],$$

$$C=F(F+1)-J(J+1)-I(I+1). \qquad (6.19)$$

Here I is a spin of nucleus, F is a full momentum of system, J is a full electron momentum. Constants of the hyperfine splitting are expressed through the standard radial integrals:

$$A=\{[(6.4{,}32587)10^{-4}Z^2\chi g_I]/(6.4\chi^2-1)\}(6.RA)_{-2},$$

$$B=\{7.2878\ 10^{-7}\ Z^3Q/[(6.4\chi^2-1)I(6.I-1)\}\ (6.RA)_{-3}, \qquad (6.20)$$

Here g_I is the Lande factor, Q is a quadruple momentum of nucleus (6.in Barn); radial integrals are defined as follows:

$$(RA)_{-2}=\int_0^\infty drr^2F(r)G(r)U(1/r^2,R),$$

$$(RA)_{-3}=\int_0^\infty drr^2[F^2(r)+G^2(r)]U(1/r^3,R) \qquad (6.21)$$

and calculated in the Coulomb units (6.=3,57 $10^{20}Z^2m^{-2}$; = 6,174 $10^{30}Z^3m^{-3}$ for valuables of the corresponding dimension). The radial parts F and G of two components of the Dirac function for electron, which moves in the potential $V(6.r,R)+U(6.r,R)$, are determined by solution of the Dirac equations (6.see

above; system (6.1)). For calculation of potentials of the hyperfine interaction $U(6.1/r^n,R)$, we solve the following differential equations:

$$U(6.1/r^n,R)=-ny(6.r,R)/r^{n+1}$$

They are analogous to the equations (6.9) and (6.10). The functions $dU(6.1/r^n,R)/dR$ are calculated within the analogous procedure. The electric quadrupole spectroscopic HFS constant B of an atomic state related to the electric field gradient q and to electric quadrupole moment eQ of the nucleus as: $B=eqQ/h$.

So, to obtain the corresponding value of Q one must combine the HFS constants data with the electric field gradient obtained in our approach from the QED PT calculation.The details of calculation are presented in [11,14, 17,18].

6.3. Results of calculation and conclusion

We have carried out the test calculation of the hyperdine structure parameters (6.plus deriviatives of the energy contribution on nuclear radius) for atom of hydrogen ^{1}H and superheavy H-like ion with nuclear charge Z=170. For hydrohen atom there are available sufficiently eact data for hyperfine splitting energiesof 1s, 2s levels. For superheavy ion Z=170 there is noe experiment and we an only compair theoretical results with the fermi function for charge distribution in a nucleus with data of analogous calculation with the gauss function for charge distribution. The electron moves in the nuclear V plus vacuum-polarization potential (6.the core potential is naturally absent). In table 1 we present the experimental [21] an theoretical (6.our test calculation) results for hyperfine splitting energies for 1s, 2s levels of hydrogen atom There is very good agreement between theiry and experiment.

In table 2 we present the results of our calculation for the hyperdine structure parameters (6.plus deriviatives of the energy contribution on nuclear radius) for the superheavy H-like ion with nuclear charge Z=170. We have used the denotations as follows:

Table 6.1. Experimental [21] an theoretical (6.our test calculation) results for hyperfine splitting energies for 1s, 2s levels of hydrogen atom

Electron term Quantum numbers of full moment	Experiment $\Delta\nu$(6.F,F'), MHz ΔE(6.F,F'), 10^{-3} cm^{-1}	Наш расчет $\Delta\nu$(6.F,F'), MHz ΔE(6.F,F'), 10^{-3} cm^{-1}
1s $^2S_{1/2}$ (6.1,0)	1420,406 47, 379	1419,685 47, 355
2s $^2S_{1/2}$ (6.1,0)	177,557 5, 923	177,480 5, 920

$$A=10^8A/Z^3g_I,(6.eV);$$
$$DA=(6.10^{-2}/Z^4g_I)(6.\partial A/\partial R),\ (6.eV/cm);$$
$$B=(6.10^7BI(6.2I-1))/Z^3Q,\ (6.eV/Barn);$$
$$DB=[(6.10^{-3}I(6.2I-1))/Z^4Q](6.\partial B/\partial R),\ (6.eV/Barn\ cm);$$
(6.22)
$$U=-(6.10^4/Z^4)<U(6.r,R)>,\ (6.eV);$$
$$DU=(6.10^{-1}/Z^5)(6.\partial<U(6.r,R)>/\partial R),\ (6.eV/cm);.$$
$$DV=[10^{-8}/Z^3](6.\partial<V>/\partial R),\ (6.eV/cm);$$

Table 6.2 Characteristics of one-electron states for H-like ion with nuclear charge Z=170 (our calculation)

	$1s_{1/2}$	$2s_{1/2}$	$2p_{1/2}$	$2p_{3/2}$	$3s_{1/2}$	$3p_{1/2}$	$3p_{3/2}$
A	4337	831	3867	1,59	207	322	0,615
DA	1039	228	941	0,0001	56,8	84,0	0,0001
B	9091	1897	8067	0,07	475	707	0,04
DB	7245	1557	6405	0,0008	395	574	0,0003
DV	1255	273	1108	0,0011	67,7	98,3	0,0005
U	1453	282	1301	1,31	69,3	109	0,62
DU	2343	503	2071	0,0015	127	185	0,0007

The detailled results of calculation of different energy contributions (6.eV) into energy of the $2s_{1/2}$-$2p_{1/2}$ transition in spectrun of the U^{89+}, calculated within different theoretical schemes: our approach (6.column F), MCDF (6.Cheng-Kim-Desclaux; A); model PT with the Dirac-Fock "0" approximation (6.Ivanov etal; B); relativistic multiparticle PT with the zeroth Hartree-Fock-Slater potential (6.Persson-Lindgren-Salomonson; C); multiparticle PT with Dirac-Fock "0" approximation (6.Blundell; D) [4-8,11,14] have been presented in ref. [12]. Though agreement between all theoretical and experimental data is in a whole quite good, more exact results are obtained by meqans of the methods (6.C) and (6.F). The results of our calculation for contributions to energy due to the the self-energy (6.SE) part of the Lamb shift and vacuum polarization correction (6.VP) of the Lamb shift for Li-like ions (6.account from core $1s^2$ energy) are also presented in ref. [12]. The detailed analysis of the VP and SE energy contributions shows that for ions with small Z the QED effects contribution is not significant, but with growth of Z (6.Z>40) a contribution of the QED became very important. Moreover for heavy and superheavy ions its account is principally important. Regarding the role of the nuclear finite size effect, let us underline that for multicharged ions with z<20 its contribution is very small, but for ions with Z>70 it can approximately be equal to the vacuum polarization contribution on absolute value. In table 3 the results of calculation of the nuclear correction into energy of the low transitions for Li-like ions are presented.

Table 6.3. Results calculation of the nuclear finite size correction into energy (6.cm^{-1}) of the low transitions for Li-like ions and values of the effective radius of nucleus (6.10^{-13} cm)

Z	$2s_{1/2}$ - $2p_{1/2}$	$2s_{1/2}$ - $2p_{3/2}$	R
20	- 15,1	- 15,5	3,26
30	- 117,5	- 118,0	3,73
41	- 659,0	- 670,0	4,14
59	- 6 610,0	- 6 845,0	4,68
69	- 20 690,0	- 21 712,0	4,93
79	- 62 315,0	- 66 931,0	5,15
92	- 267 325,0	- 288 312,0	5,42

Our calculation showed also that a variation of the nuclear radius on several persents could lead to to changing the transition energies on dozens of thousands $10^3 cm^{-1}$ We have carried out the calculation of constants of the hyperfine interaction: the electric quadruple constant *B*, the magnetic dipole constant A with inclusion of nuclear finiteness and the Uehling potential for Li-like ions. Analogous calculations of the constant A for *ns* states of hydrogen-, lithium- and sodium-like ions were made in ref. [11,22].

Table 6.4 Constants of the hyperfine electron-nuclear interaction:

$$A = Z^3 g_I \, \bar{A} \, \text{cm}^{-1}, \qquad B = \frac{Z^3 Q}{I(2I-1)} \bar{B} \ \text{cm}^{-1}$$

nlj	*Z*	20	69	79	92
2s	$\bar{A}$	93 –03	176 -02	215 -02	314 -02
3s	$\bar{A}$	26 –03	51 –03	63 –03	90 –03
4s	$\bar{A}$	15 –03	19 –03	24 –03	36 –03
$2p_{1/2}$	$\bar{A}$	25 –03	56 –03	71 –03	105 –02
$3p_{1/2}$	$\bar{A}$	81 –04	16 –03	20 –03	31 –03
$4p_{1/2}$	$\bar{A}$	32 –04	72 –04	91 –04	11 –03
$2p_{3/2}$	$\bar{A}$	50 –04	67 –04	71 –04	72 –04
	$\bar{B}$	9 –04	13 –04	15 –04	17 –04
$3p_{3/2}$	$\bar{A}$	13 –04	19 –04	21 –04	22 –04
	$\bar{B}$	31 –05	51 –05	55–05	62 –05
$4p_{3/2}$	$\bar{A}$	62 –05	89 –05	92 –05	8 –04
	$\bar{B}$	10 –05	20 –05	22 –05	26 –05
$3d_{3/2}$	$\bar{A}$	88 –05	10 –04	11 –04	12 –04
	$\bar{B}$	51 –06	9 –05	10 –05	11 –05
$4d_{3/2}$	$\bar{A}$	35 –05	51 –05	55 –05	58 –05
	$\bar{B}$	12 –06	44 –06	50 –06	56 –06
$3d_{5/2}$	$\bar{A}$	36 –05	48 –05	50 –05	52 –05
	$\bar{B}$	21 –06	38 –06	39 –06	40 –06
$4d_{5/2}$	$\bar{A}$	15 –05	19 –05	20 –05	21 –05
	$\bar{B}$	59 –07	15 –06	16 –06	17 –06

In these papers other basis's of the relativistic orbitals were used. Besides, another model for the charge distribution in the nucleus was accepted and another method of numerical calculation for the Uehling potential was used. In table 4 the calculation results for the constants of the hyperfine splitting for the lowest excited states of Li-like ions are presented. Analogous data for other states have been presented earlier (6.see ref. [12]).

In tables 5, 6 we present calculated values of deriviatives of the one-electron characteristics on nuclear radius (6.in cm^{-1}/cm) for 2l,3l,4l (6.l=0,1) states of the Li-like ions with minimally possible valus of j:

$$d\langle|V|\rangle /dR=Z^3DV \ (cm^{-1}/cm);$$

$$d\langle|U|\rangle /dR=Z^5DU \ (cm^{-1}/cm),$$

$$dA/dR=Z^4g_IDA \ (cm^{-1}/cm).$$

Here $1cm^{-1}$ is an energy unit and 1cm is a length unit. Let us remember that here V is a potential of the elctron-nuclear interaction and U is the Uehling vacuum-polarization potential. Considered value of full moment is j=3/2 for deriviative of the constant B on nuclear radius $\partial B/\partial R$ and value j=3/2 for other operators. It should be noted that the correspondimg characteristics are less sesitive to the nuclear size for states with the large valus of moment j. In any case cited effects are not observed in the modern experiment.

In table 7 we present the calculated values of deriviatives of the hfs constant B on nuclear radius (6.in cm^{-1}/cm); $dB/dR= -Z^4QDB/[I(6.2I-1)]$. Let us not that for deriviatives in tables 5,6,7 the main member of degree dependence upon a charge Z is separated. The remained Z-dependence is directly connected with relativistic and nuclear (6.the finite nuclear charge) effects in the one-electron functions.

Table 6.5. Deriviatives of the one-electron characteristics on nuclear radius (in cm^{-1}/cm) for 2s,3s,4s states of the Li-like ions: $d\langle|V|\rangle/dR=Z^3DV$, $d\langle|U|\rangle/dR=Z^5DU$, $dA/dR=Z^4g_IDA$

nlj Z		20	30	41	59	69	79	92
$2s_{1/2}$	*DV*	10 +11	20+11	41 +11	121 +12	223 +12	415 +12	967 +12
	DU	15 +06	14+06	16 +06	20 +06	25 +06	36 +06	64 +06
	DA	15 +06	19+06	24 +06	44 +06	63 +06	101 +07	197 +07
$3s_{1/2}$	*DV*	28 +10	60+10	12 +11	35 +11	65 +11	122 +12	293 +12
	DU	45 +05	42+05	44 +05	60 +05	81 +05	10 +06	18 +06
	DA	44 +05	56+05	74 +05	12 +06	18 +06	29 +06	57 +06
$4s_{1/2}$	*DV*	11 +10	24+10	51 +10	13 +11	26 +11	50 +11	121 +12
	DU	18 +05	17+05	18 +05	24 +05	32 +05	47 +05	80 +05
	DA	18 +05	23+05	30 +05	55 +05	81 +05	11 +05	23 +05

Table 6.6. Deriviatives of the one-electron characteristics on nuclear radius (in cm^{-1}/cm) for 2p,3p,4p states of the Li-like ions: $d\langle|V|\rangle/dR=Z^3DV$, $d\langle|U|\rangle/dR=Z^5DU$, $dA/dR=Z^4g_IDA$

nlj/ Z		20	30	41	59	69	79	92
$2p_{1/2}$	*D V*	31 +08	15+09	66 +09	43 +10	10 +11	29 +11	108 +12
	D U	50 +03	11+04	21 +04	72 +04	12 +05	25 +05	72 +05
	D A	55 +03	16+04	42 +04	15 +05	34 +05	78 +05	20 +06
$3p_{1/2}$	*D V*	10 +08	57+08	22 +09	14 +10	41+10	11 +11	38 +11
	D U	18 +03	39+03	84 +03	25 +04	49 +04	10 +05	25 +05
	D A	19 +03	56+03	13 +04	60 +04	12 +05	27 +05	81 +05
$4p_{1/2}$	*D V*	49 +07	25+08	10 +09	69 +09	17 +10	46 +10	16 +11
	D U	87 +02	17+03	37 +03	11 +04	21 +04	42 +04	10 +05
	D A	86 +02	24+03	67 +03	26 +04	58 +04	11 +05	34 +05

Table 6.7. Deriviatives of the hfs constant B on nuclear radius (6.in cm^{-1}/cm); $dB/dR= -Z^4QDB/[I(6.2I-1)]$.

nlj/Z		20	30	41	59	69	79	92
$2p_{3/2}$	*DB*	02 +02	05 +02	11 +02	17 +02	27 +02	40 +02	71 +02
$3p_{3/2}$	*DB*	19+01	26 +01	37 +01	57 +01	95 +01	15 +02	27 +02
$4p_{3/2}$	*DB*	03 +01	06 +01	11 +01	21 +01	38 +01	60 +02	12 +02

References

1. Glushkov A.V., Advanced Relativistic Energy Approach to Radiative Decay Processes in Multielectron Atoms and Multicharged Ions// Quantum Systems in Chemistry and Physics: Progress in Methods and Applications. Series: Progresss in Theoretical Chemistry and Physics, Eds. K.Nishikawa, J. Maruani, E.Brandas, G. Delgado-Barrio, P.Piecuch (Berlin, Springer).-2013-Vol.26.-P.231-254;
2. Khetselius O.Yu., Relativistic energy approach to cooperative electron-gamma-nuclear processes: NEET Effect// Quantum Systems in Chemistry and Physics: Progress in Methods and Applications. Series: Progresss in Theoretical Chemistry and Physics, Eds. K.Nishikawa, J. Maruani, E.Brandas, G. Delgado-Barrio, P.Piecuch (Berlin, Springer).-2012-Vol.26.-P.217-230.
3. K.G. Dyall, K. Faegri, Jr. *Introduction to Relativistic Quantum Theory* (Oxford University Press, Oxford, 2007); I.P. Grant, *Relativistic Quantum Theory of Atoms and Molecules, Theory and Computation, Springer Series on Atomic, Optical, and Plasma Physics*, vol. 40 (Springer, Berlin, 2007), p. 587–626
4. A.V. Glushkov, *Relativistic and Correlation Effects in Spectra of Atomic Systems* (Nauka, Moscow-Odessa, 2006), 550p.
5. A.V. Glushkov, *Relativistic Quantum Theory. Quantum Mechanics of Atomic Systems* (Astroprint, Odessa, 2008), 900p.
6. I.P. Grant, H.M. Quiney, Int. J. Quant. Chem**. 80**, 283–297 (2000) ; K.L. Bell, K.A. Berrington, D.S.F. Crothers, A. Hibbert, K.T. Taylor, *Bertha: 4-Component Relativistic Molecular Quantum Mechanics, in Supercomputing, Collision Processes, and Application*, Series: *Physics of Atoms and Molecules*, (Kluwer, New York, 1999) pp. 213–224.
7. M. Reiher, B. Hess, in *Modern Methods and Algorithms of Quantum Chemistry,* ed. by J. Grotendorst, John von Neumann Institute for Computing, Julich, NIC Series, vol 3, (2000) pp. 479–505.
8. H.M. Quiney, in *Relativistic Quantum Mechanics of Atoms and Molecules. New Trends in Quantum Systems in Chemistry and Physics*, Series: *Progress in Theoretical Chemistry and Physics*, vol 6 (Springer, Berlin, 2002) pp. 135–173.

9. S. Wilson, Journ. of Mol. Str.: Theochem. **547**, 279–291 (2001)
10. I.P. Grant, H.M. Quiney, Int. J. Quantum Chem. **80**, 283 (2000)
11. *Advanced Topics in Theoretical Chemical Physics*, Series: *Progress in Theoretical Chemistry and Physics*, vol. 12, ed. by J. Maruani, R. Lefebvre, E. Brändas (Springer, Berlin, 2004)
12. *H.Jensen, T.Saue, L.Visscher with contr. by V.Bakken, E.Eliav, T. Enevoldsen, T.Fleig, O.Fossgaard, T.Helgaker, J.Laerdahl, C.Larsen, P. Norman, J.Olsen, M.Pernpointner, J.Pedersen, K.Ruud, P.Salek, J. van Stralen, J.Thyssen,O. Visser, T.Winther, DIRAC Code, a relativistic ab initio electronic structure program, Release DIRAC4.0.-2004; (*http://dirac.chem.sdu.dk*).*
13. *W.*Martin, *NIST Spectra Database, version 2.0*, NIST, Washington,2004; *(http:// physics.nist.gov.asd).*
14. *C. Moore, NBS Spectra Database*, NBS, Washington, 1987.
15. A.V. Glushkov, S.V. Ambrosov, A.V. Loboda, E.P. Gurnitskaya, O.Yu. Khetselius, in *Recent Advances in Theoretical Physics and Chemistry Systems*, Series: *Progress in Theoretical Chemistry and Physics*, vol. 15, ed. by J.-P. Julien, J. Maruani, D. Mayou, S. Wilson, G. Delgado-Barrio (Springer, Berlin, 2006), pp. 285-300.
16. A.V. Glushkov, O.Yu. Khetselius, E.P. Gurnitskaya, A.V. Loboda, T.A. Florko, D.E. Sukharev, L. Lovett, in *Frontiers in Quantum Systems in Chemistry and Physics*, Series: *Progress in Theoretical Chemistry and Physics*, vol. 18, ed. by S. Wilson, P.J. Grout., J. Maruani, G. Delgado-Barrio, P. Piecuch (Springer, Berlin, 2008), p.501-522
17. A.V. Glushkov, O.Yu. Khetselius, L. Lovett, L., in: *Advances in the Theory of Atomic and Molecular Systems Dynamics, Spectroscopy, Clusters, and Nanostructures*. Series: *Progress in Theoretical Chemistry and Physics*, vol. 20, ed. by P.Piecuch, J. Maruani, G. Delgado-Barrio, S. Wilson (Springer, Berlin, 2010), pp.125-172.
18. A.V. Glushkov, S.V. Ambrosov, A.V. Loboda, Yu.G. Chernyakova, O.Yu. Khetselius, A.A. Svinarenko, Nucl. Phys. A **734**S, 21 (2004)
19. A.V.Glushkov, S.V.Malinovskaya, O.Yu. Khetselius, D.E.Sukharev, A.V.Loboda, L.Lovett, Int. Journ. of Quant.Chem. **109**, 1417 (2009).
20. *Photonic, Electronic and Atomic Collisions*, ed. by F. Aumar and H. Winter

(World Scientific, Singapore, 1997), pp.1-650.

21. M. Hehenberger, H. McIntosh, E. Brändas, Phys. Rev. A **10**, 1494 (1974).
22. E.Brändas, P. Floelich, Phys. Rev.A **16**, 2207 (1977).
23. J.C. Slater, *The Consistent Field Method for Molecules and Solids: Quantum Theory of Molecules and Solids*, vol. 4 (McGraw-Hill, New York, 1974).
24. S. Wilson, in *Recent Advances in Theoretical Physics and Chemistry Systems*, Series: *Progress in Theoretical Chemistry and Physics*, vol. 16, ed. by J. Maruani, S. Lahmar, S. Wilson, G. Delgado-Barrio (Springer, Berlin, 2007), p. 11-80.
25. S. Wilson, *Handbook on Molecular Physics and Quantum Chemistry* (Wiley, Chichester, 2003).

I. Theophilou, S. Thanos, A. Theophilou, J. Chem. Phys. **127**, 234103 (2007).

26. D.J. Dean, M. Hjorth-Jensen, K. Kowalski, P. Piecuch, M. Wloch, in *Condensed Matter Theories*, ed. by J.W. Clark, R.M. Panoff, H. Li (Nova Sci. Publishers, 2006).
27. P. Piecuch, M. Wloch, J.R. Gour, D.J. Dean, M. Hjorth-Jensen, T. Papenbrock, in *Nuclei and Mesoscopic Physics: Workshop on Nuclei and Mesoscopic Physics* WNMP 2004, AIP Conference Proceedings, vol. 995, ed. by V. Zelevinsky (American Institute of Physics, Melville, NY, 2005), p. 28.
28. W. Kohn, L.J. Sham, Phys. Rev. A **140**, 1133 (1964).
29. P. Hohenberg, W. Kohn, Phys. Rev. B **136**, 864 (1964).
30. E.G. Gross, W. Kohn, *Exchange-Correlation Functionals in Density Functional Theory* (Plenum, New York, 2005).
31. *The Fundamentals of Electron Density, Density Matrix and Density Functional Theory in Atoms, Molecules and the Solid State*, Series: *Progress in Theoretical Chemistry and Physics*, vol. 14, eds. N. Gidopoulos and S. Wilson (Springer, Berlin, 2004), p.1.
32. R.M. Dreizler, Phys. Scripta T **46**, 167 (1993).

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Підручник (на англ. мові)

д-р фіз.-мат.наук, професор Глушков О.В.
д-р фіз.-мат.наук, професор Хецеліус О.Ю.
д-р фіз.-мат.наук, професор Свинаренко А.А.

Математична фізика класичних та квантових систем , Ч.1. Квантові системи

Релятивістський енергетичний підхід у математичній фізиці радіаційних та автоіонізаційних процесів у важких скінченних фермі-системах. Ррелятивістське рівняння дірака для електрона у зовнішньому полі. Метод теорії збурень qed для розрахунку важких атомів і багатозарядних іонів (визначення базису релятивістських хвильових функцій; ядерний кінцевий розмір і радіаційні кед ефекти). Одночастинкове оптимізоване калібрувально-інваріантне представлення. Енергетичний підхід до розрахунку ймовірностей радіаційного переходу. Уявна частина секлярнох матриці. Е енергетичний підхід до розрахунку ширини автоіонізації для атомів.

Релятивістський енергетичний підхід до радіаційних та автоіонізаційних процесів у важких скінченних фермі-системах (атомів та іонів). Ймовірності радіаційного переходу та сили осцилятора для переходів у спектрах деяких важких атомів і іонів. імовірності радіаційного переходу та сили осцилятора для переходів у спектрах багатозарядних іонів. Ймовірності радіаційного переходу та автоіонізаційнї ширини для багатозарядні іони. Математична модель розпаду автоіонізаційних резонансів у слабкому електричному полі. Математичні основи лазерного фотоіонізаційного методу розділення ізотопів

Підручник (на англ. мові)
д-р фіз.-мат.наук, професор Глушков О.В.
д-р фіз.-мат.наук, професор Хецеліус О.Ю.
д-р фіз.-мат.наук, професор Свинаренко А.А.

Математична фізика класичних та квантових систем , Ч.2.

Видавець і виготовлювач
Одеський державний екологічний університет
вул. Львівська, 15, м. Одеса, 65016
тел./факс: (0482) 32-67-35
E-mail: info@odeku.edu.ua
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