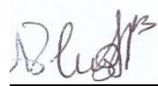


МІНІСТЕРСТВО ОСВІТИ І НАУКИ УКРАЇНИ  
ОДЕСЬКИЙ ДЕРЖАВНИЙ ЕКОЛОГІЧНИЙ УНІВЕРСИТЕТ

**Methodical instructions  
for practical work, test performance,  
distance learning of PhD students  
in the discipline “OPTICS AND SPECTROSCOPY OF  
RELATIVISTIC ATOMS AND MULTIPLE-CHARGED IONS”, Part 4  
(Training of PhD students of the specialty: 104 –  
“Physics and Astronomy” and others)**

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на засіданні групи забезпечення спеціальності  
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Methodical instructions for practical work, test performance, distance learning of PhD students in the discipline “OPTICS AND SPECTROSCOPY OF RELATIVISTIC ATOMS AND MULTIPLE-CHARGED IONS”, Part 4. (Training specialty: 104 - “Physics and Astronomy” and others)

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## PREFACE

Discipline " OPTICS AND SPECTROSCOPY OF RELATIVISTIC ATOMS AND MULTIPLE-CHARGED IONS " is an elective discipline in the cycle of professional training of postgraduate or PhD students (third level of education) in the specialty 104- Physics and Astronomys.

It is aimed at: i) K11 Ability to analyze and identify a complex of major problems in a certain field of modern physics and, in particular, optics and spectroscopy of atoms, multi-charged ions, molecular, quantum, laser systems, solids, as well as the atmosphere and ocean; Ability to develop new and improve existing methods of describing optical and spectroscopic properties of solids based on methods of quantum mechanics, quantum chemistry of solids, as well as methods of relativistic quantum theory; ii). K12 The ability to create physical, mathematical and computer models in optics and spectroscopy of physical systems with the implementation of effective algorithms and specialized software. Ability to acquire new fundamental knowledge in optics and spectroscopy of atoms, molecules, solids, laser systems, as well as geophysical systems (atmosphere and ocean). These methodical instructions are for self-studying work of the second-year PhD students and tests performance in the discipline "Quantum Geometry and Dynamics of Resonances".

Program learning outcomes include: P111 Ability to conduct research on optics and spectroscopy of atoms, multi-charged ions, molecular, quantum, laser systems, solid bodies, as well as the atmosphere and ocean in the context of existing theories, make reasoned conclusions (including assessment of the degree of uncertainty) and proposals for further research; P112 The ability to use modern or develop new approaches to the calculation of fundamental characteristics, in particular, based on methods of quantum mechanics, electrodynamics, electronics in optics and spectroscopy of atoms, molecules, solids, laser systems, as well as geophysical systems (atmosphere and ocean); P121 The ability to create physical, mathematical and computer models in the optics and spectroscopy of atoms, molecules, solids, laser systems, solids, as well as geophysical systems (atmosphere and ocean), check ix adequacy, research ix to obtain new conclusions and deepen understanding of fundamental processes in the physical system, analyzing limitations; P122 The ability to achieve relevant knowledge using effective, including new methods, models, algorithms for determining the physical (optical and spectroscopic) characteristics of atoms, molecules, solids, laser systems, as well as geophysical systems (atmosphere and ocean), processing the results of numerical and natural experiments.

The main topic of this work is a Resonance dynamics for quantum systems in an electromagnetic field. Methods for calculating energies and widths of Stark resonances (Look Syllabus of the discipline, edition 2023)

# **I. Topic: QED multiparticle perturbation theory for atoms and multicharged ions. Radiation of lower and higher orders. Lamb shift and vacuum polarization correction. (L 2.4).**

Topic: КЕД багаточастинкова теорія збурень для атомів та багатозарядних іонів. Радіаційні нижчих та вищих порядків. Зсув Лемба та поправка на поляризацію вакуума. (Л 2.4)

## **1. Introduction**

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 (c.f.[1-38]). 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 (MCDF) approximation (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  $Z$  ( $Z$  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  $1/Z$ ,  $\alpha Z$  ( $\alpha$  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 (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, including calculating the energies and constants of the hyperfine structure, derivatives of the one-electron characteristics on nuclear radius, nuclear electric quadrupole, magnetic dipole moments etc (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 (QED) perturbation theory (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 (the Superatom [11-18] and Dirac packages (DP) [22] are used; the DP using in a progress).

Our calculation scheme is based on gauge-invariant QED perturbation theory and generalized 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 (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 (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 (electrons screening, particle-hole interaction, mass operator iterations) [11-18]. The magnetic inter-electron interaction is accounted in the lowest (on  $\alpha^2$  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]. Generalized relativistic dynamical effective field nuclear model is presented in [18] (see also refs.[5,6,16]). The energies and constants of the hyperfine structure, derivatives of the one-electron characteristics on nuclear radius, nuclear electric quadrupole, magnetic dipole moments  $Q$  for atom of hydrogen  $^1\text{H}$  (test calculation), superheavy H-like ion with nuclear charge  $Z=170$ , Li-like multicharged ions with  $Z=20-100$ , neutral atoms of  $^{235}\text{U}$ ,  $^{201}\text{Hg}$  and  $^{227}\text{Ra}$  are calculated.

## **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 (more details can be found in ref.[11-18]).

### **2.1. Definition of the basis of relativistic orbitals**

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:

$$\begin{aligned}\frac{\partial F}{\partial r} + (1 + \chi)\frac{F}{r} - (\varepsilon + m - \nu)G &= 0 \\ \frac{\partial G}{\partial r} + (1 - \chi)\frac{G}{r} + (\varepsilon - m - \nu)F &= 0\end{aligned}\quad (1)$$

Here we put the fine structure constant  $\alpha = 1$ . The moment number

$$\chi = \begin{cases} -(1+1), & j > 1 \\ 1, & j < 1 \end{cases}\quad (2)$$

At large  $\chi$  the radial functions  $F$  and  $G$  vary rapidly at the origin of coordinates:

$$\begin{aligned}F(r), G(r) &\approx r^{\gamma-1} \\ \gamma &= \sqrt{\chi^2 - \alpha^2 Z^2}\end{aligned}\quad (3)$$

This involves difficulties in numerical integration of the equations in the region  $r \rightarrow 0$ . 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:

$$\begin{aligned}f' &= -(\chi + |\chi|)f/r - \alpha ZVg - (\alpha ZE_{n\chi} + 2/\alpha Z)g \\ g' &= (\chi - |\chi|)g/r - \alpha ZVf + \alpha ZE_{n\chi}f\end{aligned}\quad (4)$$

Here the Coulomb units (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 (4) has two fundamental solutions. We are interested in the solution regular at  $r \rightarrow 0$ . The boundary values of the correct solution are found by the first terms of the expansion into the Taylor series:

$$\begin{aligned}g &= (V(0) - E_{n\chi})r^{\alpha Z/(2\chi+1)}; \quad f = 1 \text{ at } \chi < 0 \\ f &= (V(0) - E_{n\chi} - 2/\alpha^2 Z^2)\alpha Z; \quad g = 1 \text{ at } \chi > 0\end{aligned}\quad (5)$$

The condition  $f, g \rightarrow 0$  at  $r \rightarrow \infty$  determines the quantified energies of the state  $E_{n\chi}$ . At correctly determined energy  $E_{n\chi}$  of the asymptotic  $f$  and  $g$  at  $r \rightarrow \infty$  are:

$$f, g \sim \exp\left(-r/n^*\right) \quad (6)$$

where  $n^* = \sqrt{1/2|E_{n\chi}|}$  is the effective main quantum number. The equations (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  $r_k \approx 30n^*$ .

## 2.2. Nuclear potential

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 (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:

$$\rho(r|R) = \left(4\gamma^{3/2}/\sqrt{\pi}\right)\exp(-\gamma r^2) \quad (7)$$

$$\int_0^{\infty} dr r^2 \rho(r|R) = 1; \quad \int_0^{\infty} dr r^3 \rho(r|R) = R$$

were  $\gamma = 4/\pi R^2$ ,  $R$  is the effective nucleus radius. The following simple dependence of  $R$  on  $Z$  assumed:

$$R = 1.60 \times 10^{-13} z^{1/3} (cm) \quad (8)$$

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:

$$V_{nucl}(r|R) = -\left(\frac{1}{r}\right) \int_0^r dr' r'^2 \rho(r'|R) + \int_r^\infty dr' r' \rho(r'|R) \quad (9)$$

It is determined by the following system of differential equations:

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

$$y'(r, R) = r^2 \rho(r, R) \quad (10)$$

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

with the boundary conditions:

$$V_{nucl}(0, R) = -4/(\pi r)$$

$$y(0, R) = 0,$$

$$\rho(0, R) = 4\gamma^{3/2} / \sqrt{\pi} = 32/R^3 \quad (11)$$

### 2.3. General Scheme of calculation for a three-electron system

Consider the Dirac-Fock type equations for a three-electron system  $1s^2nlj$ . Formally they fall into one-electron Dirac equations for the orbitals  $1s$  and  $nlj$  with the potential:

$$V(r) = 2V(r|1s) + V(r|nlj) + V_{ex}(r) + V(r|R) \quad (12)$$

$V(r|R)$  includes the electrical and the polarization potentials of the nucleus; the components of the Hartree potential:

$$V(r|i) = \frac{1}{Z} \int d\vec{r}' \rho(r|i) / |\vec{r} - \vec{r}'| \quad (13)$$

$\rho(r|i)$  is the distribution of the electron density in the state  $|i\rangle$ ,  $V_{ex}$  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

$$V(r) = V(r|1s) + V(r|nlj) \quad (14)$$

and in the equation for the  $nlj$  orbital

$$V(r) = 2V(r|1s) \quad (15)$$

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  $1s$  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 (by evaluations) does not exceed correlation corrections of the higher orders omitted in the present calculation. The relativistic potential of core (the "screening" potential)  $2V^{(1)}(r|1s) = V_{scr}$  has correct asymptotic at zero and in the infinity; at  $\alpha \rightarrow 0$  it changes to an appropriate potential constructed on the basis of non-relativistic hydrogen-like functions.

## **2.4 Calculation of the QED radiative corrections of lower and higher orders: a self-energy part of the Lamb shift and vacuum polarization correction**

Procedure for an account of the radiative QED corrections is in details given in the refs. [12,16,17]. 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 (c.f.[1,11]):

$$U(r) = -\frac{2\alpha}{3\pi r} \int_1^\infty dt \exp(-2rt/\alpha Z) \left(1 + 1/2t^2\right) \frac{\sqrt{t^2 - 1}}{t^2} \equiv -\frac{2\alpha}{3\pi r} C(g), \quad (16)$$

where  $g = \frac{r}{\alpha Z}$ . In our calculation we usually use more exact approach. The Uehling potential, determined as a quadrature (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 (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:

$$E_{SE}(H|Z, nlj) = 0.027148 \frac{Z^4}{n^3} F(H|Z, nlj) \quad (17)$$

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:

$$E_{SE}(Z, nlj) = 0.027148 \frac{\xi^4}{n^3} f(\xi, nlj) (cm^{-1}) \quad (18)$$

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  $\xi$  for the states  $nlj$  of H-like ions with the point nucleus (in accordance with the Sommerfeld 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  $\xi$  for the states  $nlj$  of Li-like ions with the finite nucleus; 4). Calculation of  $E_{SE}$  for the sought states by the formula (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  $\xi$ . A detailed evaluation of their accuracy may be made only after a complete calculation of  $E_{SE}^n(Li Z, nlj)$ . It may be stated that the above extrapolation method is more justified than using the widely spread expansions by the parameter  $\alpha Z$ .

The procedure is sufficiently simple and realized as the numerical code with using the fourth-order Runge–Kutta method of solving the differential equations (the atomic code “Superatom-Supernucleus”) [1-8].

## II. Task options for self-sufficient work

### Task Option 1.

1). Give the key definitions of a theoretical approach to definition of the energy and spectral characteristics of the heavy relativistic atoms and multicharged ions and S-matrix formalism to describe the term of different orders i) mathematical and physical essence of zeroth order approximation of the QED perturbation theory, ii) mathematical and physical essence of approximation for determination of a nuclear potential with accounting for the nuclear corrections: iii) mathematical and physical essence of the radiative corrections of lower and higher orders: a self-energy part of the Lamb shift and vacuum polarization correction, iv) calculation of the radiative corrections of lower and higher orders: a self-energy part of the Lamb shift and vacuum polarization correction, v) Scheme for calculation of spectra of heavy three-electron multicharged ions.

Explain all definitions in **the QED perturbation theory** of the heavy relativistic atoms and multicharged ions on the example of the hydrogen, helium and lithium-like ions.

2). To apply the the QED perturbation theory by Glushkov-Khetselius et al to calculation of the radiative corrections of lower and higher orders: a self-energy part of the Lamb shift and vacuum polarization correction, for the Li-like ion of **say caesium Cs**. To perform its practical realization (using Fortran Power Station, Version 4.0; PC Code: "Superatom-SuprerNucleusk" for quantum system from the first task of the option (all necessary numerical parameters should be self-taken).

### Task Option 2.

1). Give the key definitions of a theoretical approach to definition of the energy and spectral characteristics of the heavy relativistic atoms and multicharged ions and S-matrix formalism to describe the term of different orders i) mathematical and physical essence of zeroth order approximation of the **QED perturbation** theory, ii) mathematical and physical essence of approximation for determination of a nuclear potential with accounting for the nuclear corrections: iii) mathematical and physical essence of the radiative corrections of lower and higher orders: a self-energy part of the Lamb shift and vacuum polarization correction, iv) calculation of the radiative corrections of lower and higher

orders: a self-energy part of the Lamb shift and vacuum polarization correction, v) Scheme for calculation of spectra of heavy three-electron multicharged ions.

Explain all definitions in the QED perturbation theory of the heavy relativistic atoms and multicharged ions on the example of the hydrogen, helium and lithium-like ions.

2). To apply the the QED perturbation theory by Glushkov-Khetselius et al to calculation of the radiative corrections of lower and higher orders: a self-energy part of the Lamb shift and vacuum polarization correction , for the Li-like ion of **say barium Ba**. To perform its practical realization (using Fortran Power Station , Version 4.0; PC Code: “Superatom-SuprerNucleusk” for quantum system from the first task of the option (all necessary numerical parameters should be self-taken).

### **Task Option 3.**

1). Give the key definitions of a theoretical approach to definition of the energy and spectral characteristics of the heavy relativistic atoms and multicharged ions and S-matrix formalism to describe the term of different orders i) mathematical and physical essence of zeroth order approximation of the **QED perturbation** theory, ii) mathematical and physical essence of approximation for determination of a nuclear potential with accounting for the nuclear correctios: iii) mathematical and physical essence of the radiative corrections of lower and higher orders: a self-energy part of the Lamb shift and vacuum polarization correction, iv) calculation of the radiative corrections of lower and higher orders: a self-energy part of the Lamb shift and vacuum polarization correction, v) Scheme for calculation of spectra of heavy three-electron multicharged ions.

Explain all definitions in the QED perturbation theory of the heavy relativistic atoms and multicharged ions on the example of the hydrogen, helium and lithium-like ions.

2). To apply the the **QED perturbation theory** by Glushkov-Khetselius et al to calculation of the radiative corrections of lower and higher orders: a self-energy part of the Lamb shift and vacuum polarization correction , for the **Li-like ion of say galolinium Gd**. To perform its practical realization (using Fortran Power Station , Version 4.0; PC Code: “Superatom-SuprerNucleusk” for quantum system from the first task of the option (all necessary numerical parameters should be self-taken).

#### Task Option 4.

1). Give the key definitions of a theoretical approach to definition of the energy and spectral characteristics of the heavy relativistic atoms and multicharged ions and S-matrix formalism to describe the term of different orders i) mathematical and physical essence of zeroth order approximation of the **QED perturbation theory**, ii) mathematical and physical essence of approximation for determination of a nuclear potential with accounting for the nuclear corrections: iii) mathematical and physical essence of the radiative corrections of lower and higher orders: a self-energy part of the Lamb shift and vacuum polarization correction, iv) calculation of the radiative corrections of lower and higher orders: a self-energy part of the Lamb shift and vacuum polarization correction, v) Scheme for calculation of spectra of heavy three-electron multicharged ions.

Explain all definitions in the **QED perturbation theory** of the heavy relativistic atoms and multicharged ions on the example of the hydrogen, helium and lithium-like ions.

2). To apply the QED perturbation theory by Glushkov-Khetselius et al to calculation of the radiative corrections of lower and higher orders: a self-energy part of the Lamb shift and vacuum polarization correction, for the Li-like ion of **say ytterbium Yb**. To perform its practical realization (using Fortran Power Station, Version 4.0; PC Code: "Superatom-SuprerNucleusk" for quantum system from the first task of the option (all necessary numerical parameters should be self-taken).

#### Task Option 5.

1). Give the key definitions of a theoretical approach to definition of the energy and spectral characteristics of the heavy relativistic atoms and multicharged ions and S-matrix formalism to describe the term of different orders i) mathematical and physical essence of zeroth order approximation of the **QED perturbation theory**, ii) mathematical and physical essence of approximation for determination of a nuclear potential with accounting for the nuclear corrections: iii) mathematical and physical essence of the radiative corrections of lower and higher orders: a self-energy part of the Lamb shift and vacuum polarization correction, iv) calculation of the radiative corrections of lower and higher

orders: a self-energy part of the Lamb shift and vacuum polarization correction, v) Scheme for calculation of spectra of heavy three-electron multicharged ions.

Explain all definitions in the **QED perturbation theory** of the heavy relativistic atoms and multicharged ions on the example of the hydrogen, helium and lithium-like ions.

2). To apply the the QED perturbation theory by Glushkov-Khetselius et al to calculation of the radiative corrections of lower and higher orders: a self-energy part of the Lamb shift and vacuum polarization correction , for the Li-like ion of **say thullium Tm**. To perform its practical realization (using Fortran Power Station , Version 4.0; PC Code: “Superatom-SuprerNucleusk” for quantum system from the first task of the option (all necessary numerical parameters should be self-taken).

### **Task Option 6.**

1). Give the key definitions of a theoretical approach to definition of the energy and spectral characteristics of the heavy relativistic atoms and multicharged ions and S-matrix formalism to describe the term of different orders i) mathematical and physical essence of zeroth order approximation of the **QED perturbation theory**, ii) mathematical and physical essence of approximation for determination of a nuclear potential with accounting for the nuclear correctios: iii) mathematical and physical essence of the radiative corrections of lower and higher orders: a self-energy part of the Lamb shift and vacuum polarization correction, iv) calculation of the radiative corrections of lower and higher orders: a self-energy part of the Lamb shift and vacuum polarization correction, v) Scheme for calculation of spectra of heavy three-electron multicharged ions.

Explain all definitions in the **QED perturbation theory** of the heavy relativistic atoms and multicharged ions on the example of the hydrogen, helium and lithium-like ions.

2). To apply the the QED perturbation theory by Glushkov-Khetselius et al to calculation of the radiative corrections of lower and higher orders: a self-energy part of the Lamb shift and vacuum polarization correction , for the Li-like ion of **say uranium U**. To perform its practical realization (using Fortran Power Station , Version 4.0; PC Code: “Superatom-SuprerNucleusk” for quantum system from the first task of the option (all necessary numerical parameters should be self-taken).

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