


МІНІСТЕРСТВО ОСВІТИ І НАУКИ УКРАЇНИ
ОДЕСЬКИЙ ДЕРЖАВНИЙ ЕКОЛОГІЧНИЙ УНІВЕРСИТЕТ

Methodical instructions
for practical work, test performance,
distance learning of PhD students
in the discipline "Quantum Geometry
and Dynamics of Resonances", Part 8.
(Training of PhD students of the specialty: 113 –
"Applied mathematics" and others)

«Затверджено»
на засіданні групи забезпечення спеціальності
Протокол №1 від 28/08/2021 Голова групи  Хецеліус О.Ю.

«Затверджено»
на засіданні кафедри вищої та прикладної математики
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ODESSA STATE ENVIRONMENTAL UNIVERSITY**

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Part 8.**

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Methodical instructions for practical work, test performance, distance learning of PhD students in the discipline “Quantum Geometry and Dynamics of Resonances”, Part 8. (Training specialty: 113 - “Applied mathematics” and others)

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PREFACE

Discipline "Quantum geometry and dynamics of resonances" is an elective discipline in the cycle of professional training of graduate students (third level of education) in the specialty 113- Applied Mathematics.

It is aimed at mastering (providing) a number of planned competencies, including developing fundamentally new and improving existing modern computational methods and algorithms of quantum mechanics, geometry and electrodynamics to analyze, model and predict the properties of classical and quantum systems with pronounced resonant behavior.

The place of the discipline in the structural-logical scheme of its teaching: the knowledge gained in the study of this discipline is used in writing dissertations, the topics of which are related to solving quantum mechanics, geometry and electrodynamics for analysis, modeling and forecasting properties of classical and quantum systems with resonant behavior. The basic concepts of the discipline are the desired tools of an experienced specialist in the field of applied mathematics.

The purpose of studying the discipline is to master (provide) a number of competencies, in particular, mastering the modern apparatus of fractal geometry and chaos theory, the ability to develop new and improve existing mathematical methods of analysis, modeling and forecasting based on fractal geometry and elements of chaos theory of regular and chaotic dynamics (evolution) complex systems.

After mastering this discipline, the graduate student must be able to use modern existing or improved, as well as develop fundamentally new computational methods and algorithms for quantum mechanics, geometry and electrodynamics to analyze, model and predict the properties of classical and quantum systems with resonant behavior.

These methodical instructions are for the second-year PhD students and tests performance in the discipline "Quantum Geometry and Dynamics of Resonances".

The main topics: Theory of calculating the probabilities of k-photon radiation or absorption, shift and deformation of spectral lines in the field of laser radiation, energies and widths of multiphoton resonances. Effects of energy, quality, shape (Lorentz, Gaussian, soliton, etc.) of pulse, mode composition, phase shifts of laser radiation

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Торіс: Теорія обчислення ймовірностей к-фотонного випромінювання або поглинання, зсуву та деформації спектральних ліній в полі лазерного випромінювання, енергій та ширин багатифотонних резонансів. Ефекти енергетики, якості, форми (лоренцева, гаусова, солітонна тощо) імпульсу, модового складу, фазових зсувів лазерного випромінювання. **ЗБ- Л4**

1 Introduction

In this chapter we will present the fundamentals of a consistent approach in a resonant multiphoton spectroscopy of atomic system in a realistic laser field and focus on computing multiphoton resonances parameters in the atomic systems interacting with the Lorentzian, Gaussian and soliton-like shape laser pulses. The effective technique, based on the Ivanova-Ivanov method of differential equations, for computing the infinite sums in expressions for a multiphoton resonance line moments will be schematically described. We begin our consideration within an adiabatic Gell-Mann and Low formalism. In relativistic case the Gell-Mann and Low formula expresses the imaginary part of an energy shift δE through the QED scattering matrix, which includes an interaction as with a laser field as with the photon vacuum field. It results in possibility of an uniform simultaneous consideration of spontaneous and (or) induced, radiative processes and their interference. As illustration we list the results of calculation of the multi-photon resonance shifts and widths in the caesium (three-photon resonant, four-photon ionization profile; transition 6S-6F; wavelength 1059nm) atoms and compare our results with available other theoretical and experimental data. It should be noted that the analogous results for the hydrogen (three-photon resonant, four-photon ionization profile of atomic hydrogen; 1s-2p transition; wavelength =365 nm) were earlier presented [163-165,174]. In addition, we will schematically generalize our theory for the case of nuclear systems interacting with a superintense laser field, and for the first time present the quantitative estimates for the multiphoton resonance shift in the nucleus of iron ^{57}Fe .

2 Relativistic energy approach to multiphoton processes in atomic systems in laser field. Moments of radiation atomic lines

The theoretical basis of the relativistic energy approach in atomic spectroscopy was widely discussed earlier (see, e.g. [10-12, 162-190]) and here

we will focus on the key topics following to Refs. [161-168,173-175]. Let us note that 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 [35,36, 183,188]. In constructing M , the Gell-Mann and Low adiabatic formula for δE is used. In relativistic version of the Gell-Mann and Low formula δE is connected with electrodynamical scattering matrices, which includes interaction with a laser field. Naturally, in relativistic theory the secular matrix elements are already complex in the second perturbation theory (PT) order. Their imaginary parts are connected with radiation decay possibility. The total energy shift is usually presented in the form:

$$\delta E = \text{Re}\delta E + i\text{Im}\delta E, \quad (1a)$$

$$\text{Im}\delta E = -\Gamma / 2, \quad (1b)$$

where Γ is the level width (decay possibility).

As it was said, multiphoton spectroscopy of an atom in a laser field is fully determined by position and shape of the multiphoton radiation emission and absorption lines. The lines moments M_n are strongly dependent upon the laser pulse quality: intensity and mode constitution [161-168].

Let us describe the interaction “atom-laser field” by the Ivanov potential:

$$V(r,t) = V(r) \int d\omega f(\omega - \omega_0) \sum_{n=-\infty}^{\infty} \cos(\omega_0 t + \omega_0 n \tau) \quad (2)$$

Here ω_0 is the central laser radiation frequency, n is the whole number. The potential V represents the infinite duration of laser pulses with known frequency τ . Next we will consider the interaction of an atom with a single pulse. The function $f(\omega)$ is a Fourier component of the laser pulse. The condition:

$$\int d\omega f^2(\omega) = 1 \quad (3)$$

normalizes potential $V(r,t)$ on the definite energy in the pulse.

Let us consider the pulses with Lorentzian shape (the coherent 1-mode pulse):

$$f(\omega) = \beta / (\omega^2 + \Delta^2), \quad (4a)$$

the Gaussian one (the multi-mode chaotic pulse):

$$f(\omega) = \beta \exp(-\omega^2 / \Delta^2), \quad (4b)$$

where β -normalizing multiplier, and the soliton-like pulse [174]. A case of the Lorentzian shape laser pulse has been earlier studied [161-164].

Here we will focus on the case of the Gaussian shape laser pulse [173-175]. The main program results in the calculating an imaginary part of energy shift $\text{Im}\delta E_\alpha(\omega_0)$ for any atomic level as the function of the central laser frequency ω_0 . An according function has the shape of the resonance, which is connected with the transition α - s (α , s -discrete levels) with absorption (or emission) of the “ k ” number of photons. We will calculate the following quantities for the multiphoton resonance:

$$\delta\omega(s-\alpha|k) = \int d\omega \text{Im}\delta E_\alpha(\omega) (\omega - \omega_{s\alpha} / k) / N, \quad (5a)$$

$$M_n = \int d\omega \text{Im}\delta E_\alpha(\omega) (\omega - \varpi_{s\alpha} / k)^n / N, \quad (5b)$$

$$N = \int d\omega \text{Im}\delta E_\alpha(\omega), \quad (6)$$

$$\varpi_{s\alpha} = \omega_{s\alpha} + k \cdot \delta\omega(s-\alpha|k) \quad (7)$$

where N is the normalizing multiplier; $\omega_{s\alpha}$ is position of the non-shifted line for transition s - α , $\delta\omega(s-\alpha|k)$ is the line shift under k -photon absorption. As usually, the quantities M are the moments of radiation absorption or emission lines for atomic system in a laser field.

In principle, an infinitive series of M_n determine a curve of emission and absorption. Let us remember that the zeroth (a square of the absorption curve) is usually used for measurement of an oscillator strength. The first moments M_1 , M_2 and M_3 determine the atomic line centre shift, its dispersion and the asymmetry etc. The asymmetry coefficient of resonance line is defined as follows:

$$\gamma_1 = M_3 / M_2^{3/2}. \quad (8)$$

Here, for the time being, we assume that the contribution of only one resonance is taken into consideration. It should be borne in mind that in the case of random imposition of resonances, possibly of different quantumness, the shape of the line can become substantially more complex and, in order to describe it, a definition of the higher moments is required. It is worth recalling that the method of moments was used with great success in the theory of light absorption, for example, by excitons in a solid.

To determine the quantities M_n , one should need to obtain an expansion of E_α to the following PT series:

$$\delta E_\alpha = \sum \delta E_\alpha^{(2k)}(\omega_0). \quad (9)$$

According to Refs.[161-164,173], contributions of k -photon processes first appear only in the terms $\delta E^{(2k)}$. The term $\delta E^{(2k+2)}$ contains the correction of the

following approximation. Let us note that the values of the moments are calculated in the lowest second order of the PT, whose smallness parameter is proportional to V/E (where V is the amplitude of the field oscillations, and E is the characteristic energy of the electronic transitions). The non-adiabaticity parameter is proportional to V/kE (k is a quantumness of a process). Obviously, the adiabatic approach turns out to be valid at least with the same accuracy as the PT.

An external electromagnetic field shifts and broadens the atomic levels. The standard quantum approach relates complex eigenenergies $\delta E = \delta E_r + i\Gamma/2$ and complex eigenfunctions to the corresponding resonances [168-171]. The field effects drastically increase upon going from one excited level to another. The highest levels could overlap forming a “new continuum” with lowered boundary. In the case of a strong field, its potential should appear in the Dirac equations already in the zeroth-order approximation (the solution is Dirac-Volkov type function). On the other hand, it is convenient to use methods such as operator PT with included well known “distorted-waves” zeroth approximation” in the frame of the formally exact PT. In fact a physically reasonable spectrum (eigenenergies and eigenfunctions) must be chosen as the zero order, similar to the “distorted waves” method [163,168,170]. In a case of the optimal zeroth-order spectrum, the PT smallness parameter is of the order of Γ/E , where Γ and E are the field width and bound energy of the state level examined.

Next one should use the known Gell-Mann and Low adiabatic formula for δE_α with QED scattering matrix. According to Refs. [161-168], the representation of the S - matrix in the form of PT series induces the expansion for δE_α :

$$\delta E_\alpha(\omega_0) = \lim_{\gamma \rightarrow 0} \gamma \sum_{k_1 k_2 \dots k_l} c(k_1, k_2, \dots, k_l) J_\gamma(k_1, k_2, \dots, k_l), \quad (10)$$

$$J_\gamma(k_1, k_2, \dots, k_l) = \prod_{j=1}^l S_\gamma^{(k_j)}, \quad (11)$$

$$S_\gamma^{(n)} = (-1)^n \int_{-\infty}^0 dt_1 \dots \int_{-\infty}^{t_{n-1}} dt_n \langle \Psi_\alpha | V_1 V_2 \dots V_n | \Psi_\alpha \rangle, \quad (12)$$

$$V_i = \exp(iH_0 t_i) V(r_i) \exp(-iH_0 t_i) \exp(\gamma t_i). \quad (13)$$

where S_γ is QED scattering matrix, γ is an adiabatic parameter, H_0 is the unperturbed atomic hamiltonian, $c(k_1, k_2, \dots, k_n)$ are the numerical coefficients. The details of rather cumbersome transformations are presented in Refs. [164,165], where the structure of matrix elements $S_\gamma^{(n)}$ is also described. Here we only note that one may to simplify a consideration by account of the k -photon absorption contribution in the first two PT orders. In this approximation one can write [161-164]:

$$\delta E_\alpha(\omega_0) = i \lim_{\gamma \rightarrow 0} \gamma \{ 2S_\gamma^{(2)} + 4S_\gamma^{(4)} - 2S_\gamma^{(2)} S_\gamma^{(2)} \} + \quad (14)$$

$$+ \sum_{k=2}^{\infty} 2(k+1) [S_\gamma^{(2k+2)} - S_\gamma^{(2k)} S_\gamma^{(2k)}]$$

where, for example, $S_\gamma^{(2)}$ is determined as follows [163]:

$$S_\gamma^{(2)} \sim \int_{-\infty}^0 dt_1 \int_{-\infty}^0 dt_2 \exp[\gamma(t_1 + t_2)] \langle \Psi_\alpha | \exp(iH_0 t_1) V(rt_1) \cdot \exp(-iH_0 t_1) \exp(iH_0 t_2) V(rt_2) \exp(-iH_0 t_2) | \Psi_\alpha \rangle. \quad (15)$$

If we ignore the effects of interference, the multiple summation over the pulses in the matrix element J_γ can be replaced by a single one and J_γ will contain only finite and divergent terms as $1/\gamma$ (see details in Refs. [164,165]). The latter give a finite contribution to δE_α for γ tending to zero. The integrals on a laser frequency are as follows:

$$\int' d\omega_0 F(\omega_0) = \int \{ \prod_i (n_i \omega_0 - \omega_{s_i \alpha} - ir_i \Delta) \}^{-1} \quad (16)$$

$$\{ \prod_j (-n_j \omega_0 - \omega_{s_j \alpha} - ir_j \Delta) \}^{-1} (\omega_0 - \omega_{s_\alpha} / k)^n d\omega_0$$

where $n, r \geq 0$ are the whole numbers; s_i, s_j – indexes of the virtual atomic states, on which summation is fulfilled. Using the standard technique of theory of functions of a complex variable the above written integrals in Eqs. (5) can be represented as a sum of contributions of the separated poles from the upper (k -photon absorption) and the lower (k -photon emission) semiplanes. After some transformations one can get the expressions for line moments. The final results for quantities (5) for the Gaussian shape laser pulse are as follows:

$$\delta\omega(s-a|k) = [\pi\Delta / (k+1)k] [E(s, \omega_{s_\alpha} / k) - E(\alpha, \omega_{s_\alpha} / k)], \quad (17)$$

$$M_2 = \Delta^2 / k, \quad (18)$$

$$M_3 = \{ 4\pi\Delta^3 / [k(k+1)] \} [E(s, \omega_{s_\alpha} / k) - E(\alpha, \omega_{s_\alpha} / k)], \quad (19)$$

where

$$E(j, \omega_{s_\alpha} / k) = \frac{1}{2} \sum_{s_i} V_{j s_i} V_{s_i j} \left[\frac{1}{\omega_{j s_i} + \omega_{s_\alpha} / k} + \frac{1}{\omega_{j s_i} - \omega_{s_\alpha} / k} \right] \quad (20)$$

The summation in (20) is over all atomic states. The equations (17)-(20) describe the main characteristics of the radiative emission and absorption line near the resonant frequency $\omega_{s\alpha}/k$. The corresponding expressions for the Lorentzian shape laser pulse are given in Refs. [161-165]. For the soliton-like pulse it is necessary to use some approximations to simplify the expressions and perform the numerical calculation [163,173,174]. The next serious problem is calculation of the sum (20), which includes infinite summations over the complete set of unperturbed (or distorted in the zeroth approximation in a case of a strong field) atomic states. One of the most widespread methods for calculating the sums (20) is the Green function method (look below). However, as it was indicated in Refs. [161-165,168], the more preferable and effective method is based on the advanced algorithm of differential equations. It is worth to note that this method has been frequently used earlier in calculations of different atomic system energy and spectroscopic characteristics (see, e.g., [175-208]).

3. The modified Ivanova-Ivanov method of calculation of the perturbation theory second order sum

Below we present an effective approach to calculating the PT second order sums of the form (20). Its original version was proposed by Ivanova-Ivanov [182] to calculate sum of products of the interelectron interaction operator matrix elements over infinite set of virtual states, including the states of the negative continuum. An advanced version was elaborated in Ref [163-165,168,173]. The method leads the problem of calculating infinite sums to the solution of a system of the ordinary differential equations with the known boundary conditions under $r=0$. In theory of relativistic atom the solution is found in quadratures of the Dirac functions and some auxiliary functions (look below). The alternative approach was presented in Refs. [36,192-195,199-208] and the chapter 8 of this book [220].

The necessary sums can be expressed through sums of the following one-electron matrix elements:

$$S = \sum_{n_1} \langle n\chi m | V | n_1\chi_1 m_1 \rangle \langle n_1\chi_1 m_1 | V | n\chi m \rangle / (\varepsilon_{n_1\chi_1 m_1} - \varepsilon), \quad (21)$$

where $(n\mu m)$ – quantum numbers of one-electron states, $\varepsilon = \varepsilon_{n\chi m} + \omega_{s\alpha}/k$ is the energy parameter. One-electron energies $\varepsilon_{n\chi m}$ include the rest energy $(\alpha Z)^{-2}$, where α is the fine structure constant and Z is charge of a nucleus. Here and below we use the Coulomb units (1 C.u. = Z^2 a.u.e.; a.u.e. = 1 atomic unit of energy).

Let us consider schematically a procedure of calculating the sum (21) following to Refs. [162-165,182]. When calculating the resonances shifts it is necessary to determine (21) in the case of running an index n_1 over the whole spectrum of states.

For definiteness, let us concretize an interaction of atom with a laser field. In particular, for the typical dipole interaction the corresponding potential is as follows:

$$V(\mathbf{r})=(\mathbf{a},\boldsymbol{\alpha}), \quad (22)$$

where \mathbf{a} is a vector of polarization of radiation; $\boldsymbol{\alpha}$ is a vector of the Dirac matrices.

One should introduce a bi-spinor of the following form [36,161-163,182]:

$$\Psi_{\chi_1 m_1} = \sum_{n_1} \phi_{n_1 \chi_1 m_1} \langle n_1 \chi_1 m_1 | V | n \chi m \rangle / (\varepsilon_{n_1 \chi_1 m_1} - \varepsilon) \quad (23)$$

According to Refs. [161-164,167] (see also Eqs. (29),(30) in the chapter 8 of this book [220]), the radial parts F , G of a bi-spinor Ψ satisfy the system of differential equations:

$$-F' / \alpha Z + (1 + \chi_1) F / \alpha Z r + A_- G = C(\mathbf{a} | j_1 l_1 m_1, \tilde{j} \tilde{l} m) f_{n \chi} / \alpha Z, \quad (24a)$$

$$G' / \alpha Z + (1 - \chi_1) G / \alpha Z r + A_+ F = C(\mathbf{a} | j_1 l_1 m_1, \tilde{j} \tilde{l} m) g_{n \chi} / \alpha Z, \quad (24b)$$

$$A_{\pm} = U_{MF}(r) \pm 1 / (\alpha Z)^2 - \varepsilon \quad (25)$$

Here $U_{MF}(r)$ is some atomic mean-field potential (see possible expressions in Refs. [36,166,188-190]). In contrast to Refs. [162,163,166], where the known Ivanov-Ivanova potential [181] was actually used, in this paper (and also in Refs. [165,168,170,173]) we use a more general potential of the density functional theory (in the optimized form). For the one-quasiparticle atomic systems as $U_{MF}(r)$ we use the Coulomb potential of an atomic core plus the Kohn-Sham exchange and modified Lundqvist-Gunnarsson correlation potentials (see, e.g., [36, 197]).

The corresponding functions in Eqs. (24) are dependent upon polarization vector \mathbf{a} and defined in the Refs [162-165]. As usually, in the Cartesian coordinates the vector $\mathbf{a}_3=(1,0,0)$ corresponds to linear polarization, and the vectors $\mathbf{a}_1=(1,i,0)$ and $\mathbf{a}_2=(1,-i,0)$ correspond to circular polarization.

The solution of the system (24) can be represented as follows [163,168]:

$$F(r) = (\alpha Z / 2) [h_1(r) \tilde{f}(r) - h_2(r) f(r)] / (\chi^2 - \alpha^2 Z^2)^{1/2}, \quad (26a)$$

$$G(r) = (\alpha Z / 2) [h_1(r) \tilde{g}(r) - h_2(r) g(r)] / (\chi^2 - \alpha^2 Z^2)^{1/2}. \quad (26b)$$

A pair of functions (f, g) and (\tilde{f}, \tilde{g}) are two fundamental solutions of equations (23) without the right parts. The functions $h_1(r), h_2(r)$ are determined as follows:

$$h_1(r) = C(\mathbf{a}|j_1l_1m_1, \tilde{j}\tilde{l}m) \int_0^r dr' r'^2 [g_{n\chi}(r')f(r') + f_{n\chi}(r')g(r')], \quad (27a)$$

$$h_2(r) = C(\mathbf{a}|j_1l_1m_1, \tilde{j}\tilde{l}m) \int_0^r dr' r'^2 [g_{n\chi}(r')\tilde{f}(r') + f_{n\chi}(r')\tilde{g}(r')] + C_1. \quad (27b)$$

The constant C_1 in Eqs. (27) is determined as follows:

$$C_1 \sim \int_0^\infty dr r^2 [g_{n\chi}(r)\tilde{f}(r) + f_{n\chi}(r)\tilde{g}(r)]. \quad (28)$$

in the case $\varepsilon < (\alpha Z)^{-2}$, i.e. an energy lies below the boundary of ionization and does not coincide with any of the discrete eigenvalues of the Dirac equations. In the case $\varepsilon > (\alpha Z)^{-2}$ (i.e. an energy lies above the boundary of ionization) the value C_1 is determined from the following condition:

$$\lim_{r \rightarrow \infty} r^2 \int_r^{T+r} dr' r'^2 (Ff_{\varepsilon\chi_1m_1} + Gg_{\varepsilon\chi_1m_1}) = 0, \quad (29)$$

Here $\varepsilon\chi_1m_1$ is one-electron state of scattering with energy ε ; T is a period of asymptotic oscillations of the functions f, g (see details in Refs. [161-164]):

$$T = 2\pi[\varepsilon^2 - (\alpha Z)^{-2}]^{1/2}. \quad (30)$$

Other possible situations to determine C_1 , in particular, the case of coincidence of energy ε with energy of some discrete level $n_0\chi_1m_1$, are considered in refs. [162-165]. The final expression for the sum (21) can be written as follows:

$$S = \int dr r^2 [f_{n\chi_1} \cdot G(r) \cdot C(\mathbf{a}|jlm, j_1\tilde{l}_1m_1) + g_{n\chi} \cdot F(r) \cdot C(\mathbf{a}|\tilde{j}\tilde{l}m, j_1l_1m_1)]. \quad (31)$$

Above we presented a procedure to calculate the quantity (21) in the case of running an index n_1 over the whole spectrum of states. In the case, if some state n_0 is excluded from the sum (21), one should use another system of equations (24):

$$-F'/\alpha Z + (1 + \chi_1)F/\alpha Zr + A_-G = [C(\mathbf{a}|j_1l_1m_1, \tilde{j}\tilde{l}m)f_{n\chi} - g_{n_0\chi_1m_1}C_2]/\alpha Z, \quad (32a)$$

$$G'/\alpha Z + (1 - \chi_1)G/\alpha Zr + A_+F = [C(\mathbf{a}|j_1l_1m_1, \tilde{j}\tilde{l}m)g_{n\chi} - f_{n_0\chi_1m_1}C_2]/\alpha Z, \quad (32b)$$

$$C_1 = \int dr r^2 [f_{n_0\chi_1m_1}g_{n\chi m}C(\mathbf{a}|j_1l_1m_1, \tilde{j}\tilde{l}m) - g_{n_0\chi_1m_1}f_{n\chi m}C(\mathbf{a}|\tilde{j}_1\tilde{l}_1m_1, jlm)] \quad (33)$$

Then the transformations are fulfilled in the same way as described above. Finally the computational procedure results in a solution of sufficiently simple system of the ordinary differential equations for above described functions and integral (24). The alternative approach to calculating (21) is based on the using method of the Green's function of Dirac equation and presented, for example, in Refs. [35,36,174-178] in the Dirac-Kohn-Sham model of multielectron atom.

The Green's function is defined as the solution of the inhomogeneous Dirac equation:

$$(\hat{H} - \zeta)G_E(r_1 r_2) = \delta(r_1 - r_2), \quad (34)$$

where \hat{H} is the Dirac Hamiltonian, ζ is an energy parameter. The known spectral decomposition of the Green's function is as follows:

$$G(r_1 r_2 | E) = \sum_{n\chi m} \Psi_{n\chi m}(r_2) \Psi_{n\chi m}(r_1) / (E_{n\chi} - E). \quad (35)$$

where one can usually allocate partial contributions with a fixed χ (Dirac's angular quantum number), each of which is a product of the radial $G(r_1 r_2 | E, \chi)$ and angular parts. In the relativistic theory, the Green's function is a 4-component matrix:

$$G(r_1 r_2 | E, \chi) = \begin{pmatrix} \bar{F}(r_>) F(r_<) & \bar{F}(r_>) G(r_<) \\ \bar{G}(r_>) F(r_<) & \bar{G}(r_>) G(r_<) \end{pmatrix}, \quad (36)$$

where $r_>$ ($r_<$) is more (less) of r_1, r_2 . According to Ref. [36], the system of the corresponding Dirac equations for F and G component in the Dirac-Kohn-Sham approximation is as follows [36]:

$$F' = -(\chi + |\chi|)F / r + \tilde{\alpha} \cdot [V_N(r) + V^{DKS}(r) - i\xi - \tilde{\alpha}^{-2}] G, \quad (37a)$$

$$G' = (\chi - |\chi|)G / r - \tilde{\alpha} \cdot [V_N(r) + V^{DKS}(r) - i\xi + \tilde{\alpha}^{-2}] F, \quad (37b)$$

$$\tilde{F}' = -(\chi + |\chi|)\tilde{F} / r + \tilde{\alpha} \cdot [V_N(r) + V^{DKS}(r) - i\xi - \tilde{\alpha}^{-2}] \tilde{G}, \quad (38a)$$

$$\tilde{G}' = (\chi + |\chi|)\tilde{G} / r - \tilde{\alpha} \cdot [V_N(r) + V^{DKS}(r) - i\xi + \tilde{\alpha}^{-2}] \tilde{F}, \quad (38b)$$

де $\tilde{\alpha} = \alpha Z$, $V_N(r)$ is the potential of a nucleus. The functions (F, G) represent the first fundamental solution, which is regular for $r \rightarrow 0$ and singular for $r \rightarrow \infty$. Any combination $(\tilde{F}, \tilde{G}) + X r^{2|\chi|} (F, G)$ satisfies the above written equations for (\tilde{F}, \tilde{G}) and represents singular solution at zero [18,19,23]. The right chosen combination (\bar{F}, \bar{G}) for the single value of the mixing coefficient X (regular for $r \rightarrow \infty$) is second fundamental solution (\bar{f}, \bar{g}) . The corresponding condition is as follows: $(\bar{F}, \bar{G}) \sim \exp(-Ar)$, $A = (\tilde{\alpha}^{-2} + \xi^2 \tilde{\alpha}^2)^{1/2}$. The corresponding computational procedure again includes solving an ordinary differential equations system for relativistic wave functions, computing all matrix elements and so on. In concrete numerical calculations the PC "Superatom-ISAN" package (version 93) is used.

4. Task options

Task Option 1.

- 1). Give the key definitions of an relativistic energy approach (S-matrix Gell-Mann and Low formalism) to computing the energy and widths of multiphoton

resonances in spectra in some heavy atoms: i) mathematical and physical essence of relativistic energy approach, ii) calculation of the multiphoton resonances energies and widths, iii) calculation of the multiphoton transition probabilities for atomic system, iv) analysis of the role of photon-correlation effects, including the laser pulse shape.

2). Explain all definitions on the example of the concrete analysis of the a multiphoton resonances parameters for concrete atomic system (**helium** plus system on the own choice); explain a free discrete spectrum of atomic system.

3).To apply an efficient numerical algorithm for computing autoionization resonances energies and widths **in lithium**. To perform its practical realization (using Fortran Power Station , Version 4.0; PC Code: “SuperMPh” for quantum system (all necessary numerical parameters should be self-taken).

Task Option 2.

1). Give the key definitions of an relativistic energy approach (S-matrix Gell-Mann and Low formalism) to computing the energy and widths of multiphoton resonances in spectra in some heavy atoms: i) mathematical and physical essence of relativistic energy approach, ii) calculation of the multiphoton resonances energies and widths, iii) calculation of the multiphoton transition probabilities for atomic system, iv) analysis of the role of photon-correlation effects, including the laser pulse shape.

2). Explain all definitions on the example of the concrete analysis of the a multiphoton resonances parameters for concrete atomic system (**helium** plus system on the own choice); explain a free discrete spectrum of atomic system.

3).To apply an efficient numerical algorithm for computing autoionization resonances energies and widths **in sodium**. To perform its practical realization (using Fortran Power Station , Version 4.0; PC Code: “SuperMPh” for quantum system (all necessary numerical parameters should be self-taken).

Task Option 3.

1). Give the key definitions of an relativistic energy approach (S-matrix Gell-Mann and Low formalism) to computing the energy and widths of multiphoton resonances in spectra in some heavy atoms: i) mathematical and physical

essence of relativistic energy approach, ii) calculation of the multiphoton resonances energies and widths, iii) calculation of the multiphoton transition probabilities for atomic system, iv) analysis of the role of photon-correlation effects, including the laser pulse shape.

2). Explain all definitions on the example of the concrete analysis of the a multiphoton resonances parameters for concrete atomic system (**helium** plus system on the own choice); explain a free discrete spectrum of atomic system.

3).To apply an efficient numerical algorithm for computing autoionization resonances energies and widths **in rubidium**. To perform its practical realization (using Fortran Power Station , Version 4.0; PC Code: “SuperMPh” for quantum system (all necessary numerical parameters should be self-taken).

Task Option 4.

1). Give the key definitions of an relativistic energy approach (S-matrix Gell-Mann and Low formalism) to computing the energy and widths of multiphoton resonances in spectra in some heavy atoms: i) mathematical and physical essence of relativistic energy approach, ii) calculation of the multiphoton resonances energies and widths, iii) calculation of the multiphoton transition probabilities for atomic system, iv) analysis of the role of photon-correlation effects, including the laser pulse shape.

2). Explain all definitions on the example of the concrete analysis of the a multiphoton resonances parameters for concrete atomic system (**helium** plus system on the own choice); explain a free discrete spectrum of atomic system.

3).To apply an efficient numerical algorithm for computing autoionization resonances energies and widths **in magnesium**. To perform its practical realization (using Fortran Power Station , Version 4.0; PC Code: “SuperMPh” for quantum system (all necessary numerical parameters should be self-taken).

Task Option 5.

1). Give the key definitions of an relativistic energy approach (S-matrix Gell-Mann and Low formalism) to computing the energy and widths of multiphoton resonances in spectra in some heavy atoms: i) mathematical and physical essence of relativistic energy approach, ii) calculation of the multiphoton

resonances energies and widths, iii) calculation of the multiphoton transition probabilities for atomic system, iv) analysis of the role of photon-correlation effects, including the laser pulse shape.

2). Explain all definitions on the example of the concrete analysis of the a multiphoton resonances parameters for concrete atomic system (**helium** plus system on the own choice); explain a free discrete spectrum of atomic system.

3).To apply an efficient numerical algorithym for computing autoionization resonances energies and widths **in bohr**. To perform its pracrical realization (using Fortran Power Station , Version 4.0; PC Code: “SuperMPh” for quantum system (all necessary numerical parameters should be self-taken).

Task Option 6.

1). Give the key definitions of an relativistic energy approach (S-matrix Gell-Mann and Low formalism) to computing the energy and widths of multiphoton resonances in spectra in some heavy atoms: i) mathematical and physical essence of relativistic energy approach, ii) calculation of the multiphoton resonances energies and widths, iii) calculation of the multiphoton transition probabilities for atomic system, iv) analysis of the role of photon-correlation effects, including the laser pulse shape.

2). Explain all definitions on the example of the concrete analysis of the a multiphoton resonances parameters for concrete atomic system (**helium** plus system on the own choice); explain a free discrete spectrum of atomic system.

3).To apply an efficient numerical algorithym for computing autoionization resonances energies and widths **in carbon**. To perform its pracrical realization (using Fortran Power Station , Version 4.0; PC Code: “SuperMPh” for quantum system (all necessary numerical parameters should be self-taken).

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in the discipline “Quantum Geometry and Dynamics of Resonances”, Part 8.
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