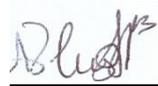МІНІСТЕРСТВО ОСВІТИ І НАУКИ УКРАЇНИ
ОДЕСЬКИЙ ДЕРЖАВНИЙ ЕКОЛОГІЧНИЙ УНІВЕРСИТЕТ

**Methodical instructions
for practical work, test performance,
distance learning of PhD students
in the discipline "QUANTUM GEOMETRY AND SPECTROSCOPY
AND DYNAMICS OF RESONANCES", Part 1.
(Training of PhD students of the specialty: 104 –
"Physics and Astronomy" and others)**

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      Methodical instructions for practical work, test performance, distance learning of PhD students in the discipline "Quantum Geometry, Spectroscopy and Dynamics of Resonances", Part 1. (Training specialty: 104 - "Physics and Astronomy" and others)

Compiler:

Glushkov O.V., D.f.-m.s.(Hab.Dr.), prof., Head of the department of mathematics and quantum mechanics(OSENU)
Khetselius O.Yu., D.f.-m.s.(Hab.Dr.), prof., prof. of the department of mathematics and quantum mechanics(OSENU)

Editor:

Glushkov O.V., D.f.-m.s.(Hab.Dr.), prof., prof. of the department of mathematics and quantum mechanics(OSENU)

PREFACE

Discipline "Quantum geometry, spectroscopy and dynamics of resonances" 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 Acquisition (providing) of a number of competencies, in particular, the achievement of relevant knowledge, understanding and the ability to use the methods of quantum geometry and dynamics of resonances, the ability to develop new and improve existing mathematical methods of analysis, modeling and forecasting based on fractal geometry and elements of the chaos theory of regular and chaotic dynamics (evolution) of complex systems, the ability to develop fundamentally new and improve existing modern computational methods and algorithms of quantum mechanics, geometry and electrodynamics for analysis, modeling and prediction of the properties of classical and quantum systems with pronounced resonant behavior. mastering the modern apparatus of fractal geometry and chaos theory.

Competencies that must be acquired or developed include; 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, solid bodies, 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".

The main topic 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: The adiabatic formalism of Gell-Mann and Lowe and the relativistic energy approach of Glushkov-Ivanov-Ivanova. Technique of moments of lines of multiphoton radiation absorption and Glushkov-Ivanov emission

Topic: Адіабатичний формалізм Гелл-Мана та Лоу і релятивістський енергетичний підхід Глушкова-Іванова-Іванової. Техніка моментів ліній багатофотонного радіаційного поглинання та випромінювання Глушкова-Іванова (Л 2.8)

1 Introduction

In this paper we will focus on theoretical studying the resonant multiphoton processes in atomic systems in an intense laser field and consider the multiphoton processes in nuclear systems. We will present a new (in comparison with above indicated methods) consistent quantum approach to atomic systems in an intense realistic laser field, based on the relativistic energy approach (S-matrix adiabatic Gell-Mann and Low formalism) and multiphoton spectral lines moments technique. In our opinion (see also, e.g., [1-31]), it is more natural and accurate to describe an atomic system interacting with a realistic laser field by means of the radiation emission and absorption spectral lines. It is important that their positions and shape fully determine a multiphoton spectroscopy of atomic system in a realistic laser pulse field. The radiation atomic lines can be described by moments of different orders M_n . Firstly, this idea was proposed by outstanding theoretical physicist Leonid Ivanov (see, e.g., [161-167]). The consistent theory of interaction of an atom with a Lorentzian shape laser pulse had been developed in Refs. [1-3].

It should be noted that the first spectral lines moments are directly linked with a field shift and width of the corresponding multiphoton resonances. It is not difficult to see that the main contribution into values of M_n is given by the resonant range. Further the values M_n can be expanded into perturbation theory (PT) series, although a perturbation theory may not be applicable for the transition probabilities in the resonant region. From the other side, application of the operator perturbation theory formalism with the physically reasonable distorted-waves approximation in the frame of the formally exact quantum-mechanical procedure can solve this problem. The development of the theory for calculation of the multiphoton lines moments in the case of the Gaussian shape laser pulse was performed in Ref. [1-8].

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 [3]. 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. [1-8]. 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. 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 matrice, 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:

$$\delta E = \mathrm{Re}\,\delta E + i\mathrm{Im}\,\delta E, \tag{1a}$$

$$\mathrm{Im}\,\delta E = -\Gamma/2, \tag{1b}$$

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:

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

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:

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

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):

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

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

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

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 $\text{Im}\delta E_\alpha$ (ω_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:

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

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

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

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

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:

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

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:

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

According to Refs.[1-6], 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. 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 [3]. 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. Thee representation of the S- matrix in the form of PT series induces the expansion for δE_α:

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

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

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

$$V_i = \exp(iH_0 t_i) V(rt_i) \exp(-iH_0 t_i) \exp(\gamma t_i). \qquad (13)$$

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. [1-3], 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 [2-4]:

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

$$\qquad (14)$$

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

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

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

$$\qquad (15)$$

$$\cdot \exp(-iH_0 t_1) \exp(iH_0 t_2) V(rt_2) \exp(-iH_0 t_2) | \Psi_\alpha \rangle.$$

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:

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

$$\{\prod_j (-n_j \omega_0 - \omega_{s_j\alpha} - ir_j\Delta)\}^{-1} (\omega_0 - \omega_{s\alpha}/k)^n d\omega_0 \qquad (16)$$

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:

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

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

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

where

$$E(j,\omega_{s\alpha}/k) = \frac{1}{2}\sum_{s_i} V_{js_i} V_{s_i j}[\frac{1}{\omega_{js_i} + \omega_{s\alpha}/k} + \frac{1}{\omega_{js_i} + \omega_{s\alpha}/k}] \qquad (20)$$

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. [3]. For the soliton-like pulse it is necessary to use some approximations to simplify the expressions and perform the numerical calculation [4]. 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. [1-8], 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.

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 [1]

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

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

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). 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 filed. In particular, for the typical dipole interaction the corresponding potential is as follows:

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

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]:

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

The radial parts F, G of a bi-spinor Ψ satisfy the system of differential equations:

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

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

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

The corresponding functions in Eqs. (24) are dependent upon polarization vector **a** and defined in the Refs [1-5]. 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:

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

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

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:

$$h_1(r) = C\left(\mathbf{a}\big| j_1 l_1 m_1, \, j\tilde{l}m\right)\int_0^r dr' r'^2 \left[g_{n\chi}(r')f(r') + f_{n\chi}(r')g(r')\right], \qquad (27a)$$

$$h_2(r) = C\left(\mathbf{a}\big| j_1 l_1 m_1, \, j\tilde{l}m\right)\int_0^r dr' r'^2 \left[g_{n\chi}(r')\tilde{f}(r') + f_{n\chi}(r')\tilde{g}(r')\right] + C_1. \qquad (27b)$$

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

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

in the case $\varepsilon < (\alpha Z)^{-2}$, i.e. an energy lies below the boundary of ionization and 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:

$$\lim_{r\to\infty} r^2 \int_r^{T+r} dr'\, r'^2 \left(Ff_{\varepsilon\chi_1 m_1} + Gg_{\varepsilon\chi_1 m_1}\right) = 0, \qquad (29)$$

Here $\varepsilon\chi_1 m_1$ 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]):

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

Other possible situations to determine C_1, in particular, the case of coincidence of energy ε with energy of some discrete level $n_0\chi_1 m_1$, are considered in refs. [3]. The final expression for the sum (21) can be written as follows:

$$S = \int dr\, r^2 \left[f_{n\chi_1} \cdot G(r) \cdot C\left(a\big| jlm, j_1\tilde{l}_1 m_1\right) + g_{n\chi} \cdot F(r) \cdot C\left(a\big| j\tilde{l}m_1, j_1 l_1 m_1\right)\right]. \qquad (31)$$

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):

$$-F'/\alpha Z + (1+\chi_1)F/\alpha Zr + A_-G = [C(\mathbf{a}|j_1l_1m_1, j\tilde{l}m)f_{n\chi} - g_{n_0\chi_1 m_1}C_2]/\alpha Z, \qquad (32a)$$

$$G'/\alpha Z + (1-\chi_1)G/\alpha Zr + A_+F = [C(\mathbf{a}|j_1l_1m_1, j\tilde{l}m)g_{n\chi} - f_{n_0\chi_1 m_1}C_2]/\alpha Z, \qquad (32b)$$

$$C_1 = \int dr\, r^2 \left[f_{n_0\chi_1 m_1} g_{n\chi m} C(a|j_1 l_1 m_1, j\tilde{l}m) - g_{n_0\chi_1 m_1} f_{n\chi m} C(a|j_1\tilde{l}_1 m_1, jlm) \right] \qquad (33)$$

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. [3-6] in the Dirac-Kohn-Sham model of multielectron atom. The Green's function is defined as the solution of the inhomogeneous Dirac equation:

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

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

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

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:

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

where $r_>$ $(r_<)$ is more (less) of r_1, r_2. According to Ref. [3], the system of the corresponding Dirac equations for F and G component in the Dirac-Kohn-Sham approximation is as follows [3]:

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

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

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

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

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 $r \to 0$ and singular for $r \to \infty$. 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 [4-6]. The right chosen combination $(\hat{F}, \hat{G})$ for the single value of the mixing coefficient X (regular for $r \to \infty$) is second fundamental solution $(\hat{f}, \hat{g})$. The corresponding condition is as follows: $(\hat{F}, \hat{G}) \sim \exp(-Ar);$, $A = (\tilde{\alpha}^{-2} + \xi^2 \tilde{\alpha}^2)^{1/2}$. 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 Some illustrative computational results

Below, as illustration, we list the results of calculation of the multi-photon resonance shifts and widths in the caesium (transition 6S-6F in the atom of Cs; wavelength 1059 nm) atom and compare our results with other available theoretical and experimental data by Zoller and Lompre et al [86,87]. The experimental studying the multi-photon ionization in Cs was carried out in Ref. [15]. Lompre et al investigated the laser temporal-coherence effects in four-photon ionization of caesium atom using a tunable wavelength Nd-glass laser pulse (the laser operated in either single or multimode; in the latter case, the laser bandwidth can be varied between $3 \cdot 10^{-2}$ and 1.5 cm^{-1}) and tuning the frequency onto the resonant three-photon transition 6S-6F. These authors showed that the resonance shift induced with incoherent laser pulses (Gaussian pulse) is statistically enhanced by a factor of 2.8±0.2 compared with the shift induced by coherent pulses (Lorenz pulse), in a physically reasonable agreement with model calculations. At the intensity $\sim 10^8$ W/cm^2 the resonance width varied linearly with the intensity and is statistically enhanced. According to [87], a line shift is linear with respect to laser intensity I (I is increased from 1,4 to $5,7 \cdot 10^7$ W/cm^2) and is equal (for Gaussian multi-mode pulse): $\delta\omega(s\alpha/k) = bI$ with $b = (5,6 \pm 0,3)$ cm^{-1}/GW·cm^{-2} (b is expressed in terms of energy of the three-photon transition 6S-6F). The corresponding shift obtained with coherent (1-mode) pulse is as follows: $\delta\omega_0(s\alpha/k) = aI$, $a = 2$ cm^{-1}/GW·cm^{-2}.

Theoretical values, obtained with using no-optimized atomic basis set (see, e.g., [167,175]), are as follows: i). for soliton-like laser pulse: $\delta\omega(s\alpha|k) = bI$ with $b=6,7$ cm^{-1}/GW·cm^{-2}; ii). for the Gaussian multi-mode pulse (chaotic light): $\delta\omega(s\alpha|k)=bI$ with $b=5.8$ cm^{-1}/GW·cm^{-2} ; iii). for the coherent one-mode pulse: $\delta\omega(s\alpha|k)=aI$, $a=2,1$ cm^{-1}/GW·cm^{-2} . The analogous theoretical values, obtained in our calculation, are as follows: a). the Gaussian pulse (chaotic light) $\delta\omega(s\alpha|k)=bI$, $b=5.63$ cm^{-1}/GW·cm^{-2}; b). the coherent one-mode pulse: $\delta\omega(s\alpha|k)=aI$, $a=2.02$ cm^{-1}/GW·cm^{-2}. One can see that for the multi-mode pulse, the radiation line shift is significantly larger (in ~ 3 times) than the corresponding shift, which is obtained for single-mode pulse.

In figure 1 we present the results of calculation for the multi-photon resonance width for transition 6S-6F in Cs in dependence on I.
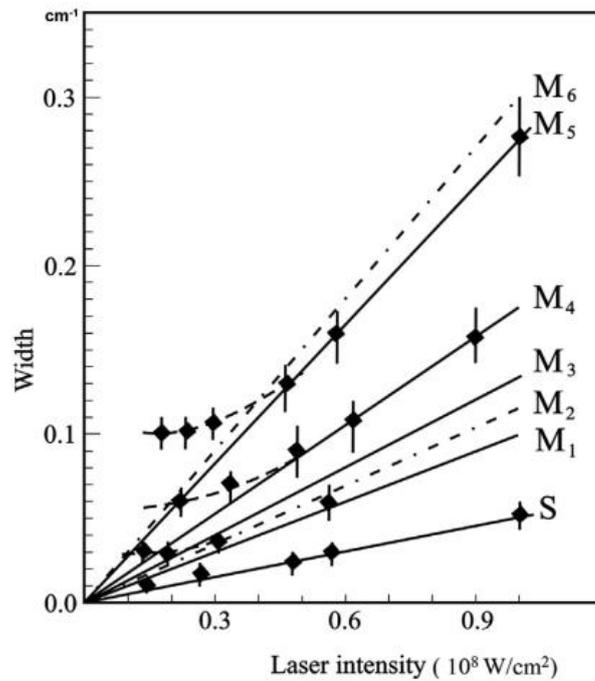

Figure 1. The multi-photon 6S-6F resonance width for Cs in dependence on the laser intensity I: S- for the single-mode Lorentzian pulse; M_1, M_3, M_4,M_5 for the multi-mode Gaussian pulse respectively with the line band 0.03, 0.055, 0.08, 0.15cm^{-1}; M_2, M_6- for the multi-mode Gaussian pulse respectively with the line band 0.03, 0.15cm^{-1} (no-optimized atomic basis set); dots-experiment (see text).

In Ref. [1] there are presented experimental data for laser pulse of the Gaussian shape with line band respectively 0.03cm^{-1}, 0.08cm^{-1}, 0.15cm^{-1}. In general there is a physically reasonable agreement between the theoretical results and experimental data. Analysis shows that the shift and width of the multi-photon resonance line for the interaction "atom- a multimode laser pulse

(chaotic light)" is greater than the corresponding shift and width for a case of the "atom- single-mode pulse (coherent light) interaction" (the Lorentzian pulse model). From the physical point of view it is provided by action of the photon-correlation effects and influence of the laser pulse multi-modity. The corresponding asymmetric nature of the multiphoton resonance line in the ^{133}Cs atom is naturally explained within the presented theoretical approach.

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 multiphoton resonances using the standard quantum-mechanical amplitude approach and new S-matrix formalism by Glushkov-Ivanov: i) mathematical and physical essense of quantum-mechanical amplitude approach , ii) mathematical and physical essense of S-matrix formalism by Glushkov-Ivanov: iii) calculation of the AC Stark effect multiphoton Stark resonances energies and widths s, iv) calculation of the ionization cross section in a presence of AC electric field, v) analysis of the role of correlation effects and value of the field strength,

Explain all definitions in theory of multiphoton resonances for atomic systems in AC electromagnetic field on the example of the hydrogen, helium and any alkali atom , preliminarily describing the corresponding spectrum of a free system , i.e. without an external electric field.

2).To apply the operator perturbation theory by Glushkov-Ivanov for computing theAC multiphoto n resonances energies and widths of any alkali atom, say **lithium Li.** To perform its pracrical realization (using Fortran Power Station , Version 4.0; PC Code: "Superatom-Stark" 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 multiphoton resonances using the standard quantum-mechanical amplitude approach and new S-matrix formalism by Glushkov-Ivanov: i) mathematical and physical essense of quantum-mechanical amplitude approach , ii) mathematical and physical essense of S-matrix

formalism by Glushkov-Ivanov: iii) calculation of the AC Stark effect multiphoton Stark resonances energies and widths s, iv) calculation of the ionization cross section in a presence of AC electric field, v) analysis of the role of correlation effects and value of the field strength,

Explain all definitions in theory of multiphoton resonances for atomic systems in AC electromagnetic field on the example of the hydrogen, helium and any alkali atom , preliminarily describing the corresponding spectrum of a free system , i.e. without an external electric field.

2).To apply the operator perturbation theory by Glushkov-Ivanov for computing theAC multiphoto n resonances energies and widths of any alkali atom, say **sodium Na.** To perform its pracrical realization (using Fortran Power Station , Version 4.0; PC Code: "Superatom-Stark" 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 multiphoton resonances using the standard quantum-mechanical amplitude approach and new S-matrix formalism by Glushkov-Ivanov: i) mathematical and physical essense of quantum-mechanical amplitude approach , ii) mathematical and physical essense of S-matrix formalism by Glushkov-Ivanov: iii) calculation of the AC Stark effect multiphoton Stark resonances energies and widths s, iv) calculation of the ionization cross section in a presence of AC electric field, v) analysis of the role of correlation effects and value of the field strength,

Explain all definitions in theory of multiphoton resonances for atomic systems in AC electromagnetic field on the example of the hydrogen, helium and any alkali atom , preliminarily describing the corresponding spectrum of a free system , i.e. without an external electric field.

2).To apply the operator perturbation theory by Glushkov-Ivanov for computing theAC multiphoto n resonances energies and widths of any alkali atom, say **rubidium Rb .** To perform its pracrical realization (using Fortran Power Station , Version 4.0; PC Code: "Superatom-Stark" 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 multiphoton resonances using the standard quantum-mechanical amplitude approach and new S-matrix formalism by Glushkov-Ivanov: i) mathematical and physical essense of quantum-mechanical amplitude approach , ii) mathematical and physical essense of S-matrix formalism by Glushkov-Ivanov: iii) calculation of the AC Stark effect multiphoton Stark resonances energies and widths s, iv) calculation of the ionization cross section in a presence of AC electric field, v) analysis of the role of correlation effects and value of the field strength,

Explain all definitions in theory of multiphoton resonances for atomic systems in AC electromagnetic field on the example of the hydrogen, helium and any alkali atom , preliminarily describing the corresponding spectrum of a free system , i.e. without an external electric field.

2).To apply the operator perturbation theory by Glushkov-Ivanov for computing theAC multiphoto n resonances energies and widths of any alkali atom, say **caesium Cs.** To perform its pracrical realization (using Fortran Power Station , Version 4.0; PC Code: "Superatom-Stark" 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 multiphoton resonances using the standard quantum-mechanical amplitude approach and new S-matrix formalism by Glushkov-Ivanov: i) mathematical and physical essense of quantum-mechanical amplitude approach , ii) mathematical and physical essense of S-matrix formalism by Glushkov-Ivanov: iii) calculation of the AC Stark effect multiphoton Stark resonances energies and widths s, iv) calculation of the ionization cross section in a presence of AC electric field, v) analysis of the role of correlation effects and value of the field strength,

Explain all definitions in theory of multiphoton resonances for atomic systems in AC electromagnetic field on the example of the hydrogen, helium and any alkali atom , preliminarily describing the corresponding spectrum of a free system , i.e. without an external electric field.

2).To apply the operator perturbation theory by Glushkov-Ivanov for computing theAC multiphoto n resonances energies and widths of any alkali atom, say **francium Fr.** To perform its pracrical realization (using Fortran Power Station , Version 4.0; PC Code: "Superatom-Stark" 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 Stark resonances using the standard quantum-mechanical amplitude approach and new formalism of operator perturbation theory by Glushkov-Ivanov: i) mathematical and physical essense of quantum-mechanical amplitude approach , ii) mathematical and physical essense of operator perturbation theory by Glushkov-Ivanov: iii) calculation of the Stark resonances energies and widths s, iv) calculation of the ionization cross section in a presence of DC electric field, v) analysis of the role of correlation effects and value of the field strength; Explain all definitions in theory of Stark resonances for atomic systems in DC electric field on the example of the hydrogen, helium and any alkali atom, preliminarily describing the corresponding spectrum of a free system , i.e. without an external electric field.

2).To apply the operator perturbation theory by Glushkov-Ivanov for computing the Stark resonances energies and widths of any alkali atom, say **Fr.** To perform its pracrical realization (using Fortran Power Station , Version 4.0; PC Code: "Superatom-Stark" for quantum system from the first task of the option (all necessary numerical parameters should be self-taken).

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