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 3.

(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 3. Zeeman Resonances (Training specialty: 104 - "Physics and Astronomy" and others)

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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 Astronomy.

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: Theory of the Zeeman effect for atoms (hydrogen and others) in a magnetic field. The Glushkov-Ivanov perturbation theory method. An atom in the intersection of electric and magnetic fields

Topic: Теорія ефекта Зеємана для атомів (водень та інші) в магнітному полі. Метод операторної теорії збурень Глушкова-Іванова. Атом у скрещениях електричному та магнітному полях (Л2.5б)

1. Introduction

In this work spectroscopy of atoms in the magnetic field as well as in the crossed external electric and magnetic fields is investigated on the basis of the operator perturbation theory. As a novel element within the operator perturbation theory, we use more flexible functions for model function, which imitates an electric field. In a case of the crossed electric and magnetic fields we develop more effective finite differences numerical scheme. As illustration, some advanced data for the hydrogen atom in the electric and crossed external electric and magnetic fields are listed. Advanced data for hydrogen atom are listed.

From the standard quantum mechanics it is well known that the external electric field shifts and broadens the bound state atomic levels. One should note that the usual quantum-mechanical approach relates complex eigen-energies (EE) $E=E_r+0,5iG$ and complex eigen-functions (EF) to the shape resonances [1-6]. The calculation difficulties in the standard quantum mechanical approach are well known and described in many Refs. Let us remind that the usual quasiclassical WKB approximation overcomes these difficulties for the states, lying far from "new continuum " boundary and, as rule, is applied in the case of a relatively weak electric field. The same is regarding the widespread asymptotic phase method (c.f.[2]). Quite another calculation procedures are used in the Borel summation of the divergent perturbation theory (PT) series and in the numerical solution of the difference equations following from expansion of the wave function over finite basis [2,3,9,10].

Experimental observation of the Stark effect in a constant (DC) electric field near threshold in hydrogen and alkali atoms led to the discovery of resonances extending into the ionization continuum (c.f.[1]). Calculation of the characteristics of these resonances as well as the Stark resonances in the strong electric field and crossed electric and magnetic fields remains very important problem of as modern atomic physics [1-51].

In this paper we go on our studying of sspectroscopy of atoms in the crossed external electric and magnetic fields. Our method of studying is based on the known formalism of the operator perturbation theory (OPT) [1-3]. According to [1-5], the essence of operator perturbation theory approach is the inclusion of the well known method of "distorted waves approximation" in the frame of the formally exact perturbation theory. As a novel element within the operator perturbation theory, we use more flexible functions for model function, which imitates an electric field. In a case of the crossed electric and magnetic fields we develop more effective finite differences numerical scheme. As illustration, some advanced data for the hydrogen atom in the electric and crossed external electric and magnetic fields are listed.

2. Method of the Glushkov-Ivanov operator perturbation theory

As our approach to strong field DC Stark effect was presented in a series of papers (see, for example, [1-6]), here we are limited only by the key aspects. According to [2,3], the Schrödinger equation for the electronic eigen-function taking into account the uniform DC electric field (the field strength is F)and the field of the nucleus (Coulomb units are used: a unit is $h^2/Ze^2 m$ and a unit of $mZ^2 e^4/h^2$ for energy) looks like:

$$[-(1 - N/Z) / r + F z - 0,5\Delta - E]\ \psi = 0 \quad (1)$$

where E is the electronic energy, Z — charge of nucleus, N — the number of electrons in atomic core. Our approach allow to use more adequate forms for the core potential (c.f.[25-27]). According to standard quantum defect theory (c.f.[3]), relation between quantum defect value μ_l, electron energy E and principal quantum number n is: $\mu_l=n-z^*(-2E)^{-1/2}$. As it is known, in an electric field all the electron states can be classified due to quantum numbers: n, n_1, n_2, m (principal, parabolic, azimuthal: $n=n_1+ n_2+m+1$). Then the quantum defect in the parabolic co-ordinates $\delta(n_1n_2m)$ is connected with the quantum defect value of the free $(F=0)$ atom by the following relation [3]:

$$\delta(n_1n_2m)=(1/n)\sum_{l=m}^{n-1}(2l+1)(C^{JM}_{J,M-m;lm})^2\mu_l$$

$$J=(n-1)/2,\ \ M=(n_1-n_2+m)/2;$$

After separation of variables, equation (1) in parabolic co-ordinates could be transformed to the system of two equations for the functions *f and g*:

$$f'' + \frac{|m|+1}{t} f' + [0{,}5E + (\beta_1 - N/Z) / t - 0{,}25\, F(t)\ t\,]\, f = 0 \qquad (2)$$

$$g'' + \frac{|m|+1}{t} g' + [0{,}5E + \beta_2 / t + 0{,}25\, F(t)\ t\,]\, g = 0 \qquad (3)$$

coupled through the constraint on the separation constants: $\beta_1 + \beta_2 = 1$.

For the uniform electric field $F(t) = F$. In ref. [11], the uniform electric field ε in (3) and (4) was substituted by model function F(t) with parameter τ ($\tau = 1.5\ t_2$) . To simplify the calculation procedure, the uniform electric field ε in (3) and (4) should be substituted by the function [57,58]:

$$\varepsilon(\mathrm{t}) = \frac{1}{t}\,\varepsilon\left[(t-\tau)\frac{\tau^4}{\tau^4+t^4}+\tau\right] \qquad (4)$$

th sufficiently large τ (τ=1.5t_2). The function $\varepsilon(t)$ practically coincides with the constant ε in the inner barrier motion region ($t<t_2$) and disappears at $t>>t_2$. Potential energy in equation (4) has the barrier. Two turning points for the classical motion along the η axis, t_1 and t_2 , at a given energy E are the solutions of the quadratic equation ($\beta = \beta_1, E = E_0$). According to [1-3], one should know two zeroth order EF of the H_0: bound state function Ψ_{Eb} (ε, ν, φ) and scattering state function Ψ_{Es} (ε, η, φ) with the same EE in order to calculate the width G of the concrete quasi-stationary state in the lowest PT order. Firstly, one would have to define the EE of the expected bound state. It is the well known problem of states quantification in the case of the penetrable barrier. Further one should solve the system (2, 3) system with the total Hamiltonian H using the conditions [11]:

$$f(t) \to 0 \text{ at } t \Rightarrow \infty$$

$$\partial x(\beta, E) / \partial E = 0 \qquad (5)$$

with

$$x(\beta, E) = \lim_{t\Rightarrow\infty} [\, g^2(t) + \{g'(t) / k\}^2\,]\, t^{|m|+1}.$$

These two conditions quantify the bounding energy E, with separation constant β_1 . The further procedure for this two-dimensional eigenvalue problem results in solving of the system of the ordinary differential equations(2, 3) with probe pairs of E, β_1. The bound state EE, eigenvalue β_1 and EF for the zero order Hamiltonian H_0 coincide with those for the total Hamiltonian H at $\varepsilon \Rightarrow 0$, where all the states can be classified due to quantum numbers: n, n_1, l , m (principal, parabolic, azimuthal) that are connected with E, β_1, m by the well known expressions.. The scattering states' functions must be orthogonal to the above defined bound state functions and to each other. According to the OPT ideology [11,12], the following form of $g_{E's}$:is possible:

$$g_{E's}(t) = g_1(t) - z_2' g_2(t) \tag{6}$$

with $f_{E's}$, and $g_1(t)$ satisfying the differential equations (2) and (3). The function g_2(t) satisfies the non-homogeneous differential equation, which differs from (3) only by the right hand term, disappearing at $t \Rightarrow \infty$.

In Ref, [7] it has been presented approach, based on solution of the 2-dimensional Schrödinger equation for an atomic system in crossed fields and operator perturbation theory. For definiteness, we consider a dynamics of the complex non-coulomb atomic systems in a static magnetic and electric fields. The hamiltonian of the multi-electron atom in a static magnetic and electric fields is (in atomic units) as follows:

$$I = 1/2(p_\rho^2 + l_z^2/\rho^2) + Bl_z/2 + (1/8)B^2\rho^2 + \\ (1/2)p_z^2 + Fz + V(r) \tag{7}$$

where the electric field F and magnetic field B are taken along the z-axis in a cylindrical system; In atomic units: 1 a.u.B=2.35·10^5T, 1a.u.F=5,144·10^6 kV/cm. For solution of the Schrödinger equation with hamiltonian equations (7) we constructed the finite differences scheme which is in some aspects similar to method [7]. An infinite region is exchanged by a rectangular region: $0<\rho<L_\rho$, $0<z<L_z$. It has sufficiently large size; inside it a rectangular uniform grid with steps h_ρ, h_z was constructed. The external boundary condition, as usually, is: $(\partial\Psi/\partial n)_r = 0$. The knowledge of the asymptotic behaviour of wave function in the infinity allows to get numeral estimates for L_ρ, L_z. A wave function has an asymptotic of the kind as: $exp[-(-2E)^{1/2}r]$, where $(-E)$ is the ionization energy from stationary state to lowest Landau level. Then L can be estimated as $L \sim 9(-2E)^{-1/2}$. The more exact estimate is found empirically. The finite-difference scheme is constructed as follows. The three-point symmetric differences scheme is used for second derivative on z. The derivatives on ρ are approximated by

(2*m*+1)-point symmetric differences scheme with the use of the Lagrange interpolation formula differentiation. To calculate the values of the width G for resonances in atomic spectra in an electric field and crossed electric and magnetic field one can use the modified operator perturbation theory method (see details in ref.[10,20]). Note that the imaginary part of the state energy in the lowest PT order is: $\mathrm{Im}E = G/2 = \pi < \Psi_{Eb} | H | \Psi_{Es} >^2$. with the total Hamiltonian of system in an electric and magnetic field. The state functions Ψ_{Eb} and Ψ_{Es} are assumed to be normalized to unity and by the δ(k -k')-condition, accordingly. Other calculation details can be found in ref. [7]. Different application are considered in Refs. [21-57].

3. Illustration results and conclusion

As an illustration,, we make computing the energy of the ground state of the hydrogen atom in crossed fields and compare results with data obtained within analytical perturbation theory by TurbinerV (see. [8]) for the case of sufficiently weak fields. Table 1 shows the values of the energy of the ground state of the hydrogen atom (the following designations: $E+E^{||}$ - energy for the case of the electric and magnetic fields are parallel; $E+E^{\perp}$ corresponds to the case of the electric and magnetic fields are perpendicular).

Table 1. Energy values (Ry) of the H ground state in electric *F* (1au=5.14·10^9 V/cm) and magnetic *B* (1 au.B=2.35·10^5 T) fields

F, *B* 10^{-2}	$E+E^{\|\|}$ Turbiner theory	$E+E^{\|\|}$ Turbiner theory	F, B 10-2	$E+E^{\|\|}$ Glushkov-Ivanov Theory	$E+E^{\perp}$ Turbiner theory
0,0	-1,000000	-1,000000	0,0	-1,000000	-1,000000
0,1	-1,000004	-1,000004	0,1	-1,000004	-1,000004
0,5	-1,000099	-1,000099	0,5	-1,000100	-1,000099
1,0	-1,000402	-1,000401	1,0	-1,000402	-1,000401
1,5	-1,000906	-1,000905	1,5	-1,000906	-1,000905
2,0	-1,001617	-1,001616	2,0	-1,001617	-1,001616
2,5	-1,002542	-1,002540	2,5	-1,002541	-1,002535
3,0	-1,003685	-1,003682	3,0	-1,003684	-1,003673
3,5	-1,005054	-1,005053	3,5	-1,005054	-1,005036
4,0	-1,0066619	-1,006659	4,0	-1,006686	-1,006627
4,5	-1,008520	-1,008517	4,5	-1,008519	-1,008464
5,0	-1,010642	-1,010636	5,0	-1,010638	-1,010556

Since the considered electric field is sufficiently weak, difference between all data in Table 1 is quite little. At the same time it is clear that the perturbation theory in the standard quantum-mechanical version is correct exclusively for the weak fields, while for strong fields it can lead to substantially inaccurate data. Really, in Table 2 we list the results for the Stark resonances energies and widths of the ground state hydrogen atom in the DC field with the strength ε=0.1 and 0.8 a.u., obtained within the most exact alternative methods and our data (see [2]).

Table 2. The energies and widths of the Stark resonances of the H ground state (F=0.1, 0.8 a.u.). Notation: (A) Hehenberger, H.V. McIntosh and E. Brändas, (B) Farrelly and Reinhardt, (C) Rao, Liu and Li [18], (D) Glushkov-Ivanov, the standard OPT method; (E)- Popov et al; (F) – our data

F, a.u.	Method	Er, a.u.	Γ/2, a.u.
0.10	A	-0.52743	$0.725 \cdot 10^{-2}$
	C	-0.527418	$0.7269 \cdot 10^{-2}$
	D	-0.527419	$0.2269 \cdot 10^{-2}$
	E	-0.527	$0.227 \cdot 10^{-2}$
	F	-0.527418	$0.7269 \cdot 10^{-2}$
0.80	B	-0.6304	0.5023
	C	-0.630415	0.50232
	D	-0.630416	0.50232
	F	-0.630415	0.50231

The comparison of our data (Table 2: F) with earlier similar results, obtained within the summation of divergent PT series, the numerical solution with expansion of the wave function over finite basis, a complex scaling plus B-spline calculation, the standard OPT one (Table 2: A-E) shows quite acceptable agreement. We believe that the OPT method with new elements will be especially efficient for atoms in the strong crossed electric and magnetic fields, where the standard methods (usual perturbation theory etc) deal with great principal and computational problems). 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-ISAN-Stark”).

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 **Zeemane 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 Zeeman and mixed resonances energies and widths s, iv) calculation of the ionization cross section in a presence of DC magnetic field, v) analysis of the role of correlation effects and value of the field strength,

Explain all definitions in theory of **Zeeman** resonances for atomic systems in magnetic 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 magnetic field

2).To apply the operator perturbation theory by Glushkov-Ivanov for computing the **Zeeman resonances** energies and widths of any alkali atom, say **sodium Na.** Consaide the case of mixed electric and magnetic field. 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 **Zeemane 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 Zeeman and mixed resonances energies and widths s, iv) calculation of the ionization cross section in a presence of DC magnetic field, v) analysis of the role of correlation effects and value of the field strength, Explain all definitions in theory of **Zeeman** resonances for atomic systems in magnetic 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 magnetic field

2).To apply the operator perturbation theory by Glushkov-Ivanov for computing the **Zeeman resonances** energies and widths of any alkali atom, say **lithium Li.** Consaide the case of mixed electric and magnetic field. 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 **Zeemane 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 Zeeman and mixed resonances energies and widths s, iv) calculation of the ionization cross section in a presence of **DC magnetic field**, v) analysis of the role of correlation effects and value of the field strength,

Explain all definitions in theory of **Zeeman** resonances for atomic systems in magnetic 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 magnetic field

2).To apply the operator perturbation theory by Glushkov-Ivanov for computing the **Zeeman resonances** energies and widths of any alkali atom, say **rubidum Rb.** Consaide the case of mixed electric and magnetic field. 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 Zeemane 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 Zeeman and mixed resonances energies and widths s, iv) calculation of the ionization cross section in a presence of DC magnetic field, v) analysis of the role of correlation effects and value of the field strength,

Explain all definitions in theory of **Zeeman** resonances for atomic systems in magnetic 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 magnetic field

2).To apply the operator perturbation theory by Glushkov-Ivanov for computing the **Zeeman resonances** energies and widths of any alkali atom, say **K.** Consaide the case of mixed electric and magnetic field. 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 Zeemane 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 **Zeeman and mixed resonances** energies and widths s, iv) calculation of the ionization cross section in a presence of DC magnetic field, v) analysis of the role of correlation effects and value of the field strength,

Explain all definitions in theory of Zeeman resonances for atomic systems in magnetic 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 magnetic field

2).To apply the operator perturbation theory by Glushkov-Ivanov for computing the **Zeeman resonances** energies and widths of any alkali atom, **caseium Cs.** Consaide the case of mixed electric and magnetic field. 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 **Zeemane 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 Zeeman and mixed resonances energies and widths s, iv) calculation of the ionization cross section in a presence of **DC magnetic field**, v) analysis of the role of correlation effects and value of the field strength,

Explain all definitions in theory of **Zeeman resonances** for atomic systems in magnetic 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 magnetic field

2).To apply the operator perturbation theory by Glushkov-Ivanov for computing the **Zeeman resonances** energies and widths of any alkali atom, say **francium Fr.** Consaide the case of mixed electric and magnetic field. 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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