

A. V. Glushkov

Odessa State Environmental University, 15, Lvovskaya str., Odessa, Ukraine
e-mail: dirac13@mail.ru

OPERATOR PERTURBATION THEORY TO HYDROGEN ATOM IN A STRONG DC ELECTRIC FIELD

A consistent uniform quantum approach to the solution of the non-stationary state problems including the DC strong-field Stark effect and also scattering problem is presented. It is based on the operator form of the perturbation theory for the Schrödinger equation. The method includes the physically reasonable distorted-waves approximation in the frame of the formally exact quantum-mechanical procedure. The zero-order Hamiltonian possessing only stationary states is determined only by its spectrum without specifying its explicit form. The method allows calculating the resonance complex energies and widths plus a complete orthogonal complementary of the scattering state functions. The calculation results of the Stark resonance energies and widths for the hydrogen atom are presented and compared with other theoretical data.

1. Introduction

The Stark effect [1] is one of the best known problems in quantum mechanics, but at the same time one of the most difficult (outside the weak-field region) [1-8]. A new interest in this effect has been stimulated in the last two decades. A range of the interesting phenomena to be studied includes: quasi-discrete state mixing; a zoo of the Landau-Zener anticrossings in non-hydrogenic (non-H) atoms; autoionization in non-H atoms; the effects of potential barriers (shape resonances); new kinds of resonances above threshold etc [1-63]. The dielectronic recombination involves highly excited (Rydberg) atomic states, which are very strongly affected by relatively weak fields [3-6]. In fact these states provide the gateway for ion-electron recombination processes. Now it is well known that weak-field effects on Rydberg states can cause the large changes in electron-ion collision cross sections. One subject stands out quite clearly: possible non-perturbative effects of the electric fields on the autoionization states responsible for dielectronic recombination. It is of a great importance for a consistent treating the different processes in a laser plasma, astrophysical environments etc [4-14]. Naturally in the last two decades a great progress has been made on

the Stark effect for the hydrogen atom as well as for non-H atoms [2-62].

An external electric field shifts and broadens the bound state atomic levels. The standard quantum-mechanical approach relates complex eigenenergies (EE) $E = E_r + i\Gamma/2$ and complex eigenfunctions (EF) to the shape resonances. The field effects drastically increase upon going from one excited level to another. The highest levels overlap forming a "new continuum" with lowered boundary. The calculation difficulties inherent to the standard quantum mechanical approach are well known. Here one should mention the well-known Dyson phenomenon. The Wentzel-Kramers-Brillouin (WKB) approximation overcomes these difficulties for the states lying far from the "new continuum" boundary. Some modifications of the WKB method [4,8,50,65,66] are introduced in Stebbings and Dunning (1983), Kondratovich and Ostrovsky (1982, 1984), Popov et al (1988, 1990) and Glushkov, Ivanov and Letokhov (1975, 1992), where the first theoretical estimation of the effectiveness of the selective ionization of the Rydberg atom using electric and laser fields has been fulfilled. The usual WKB approximation applicability is substantiated in the case of a relatively weak electric field [2,3]. One can show that the standard form of the WKB method

applicability condition can be reformulated as the requirement that the examined resonances be well separated one from other. The same is so regarding the widespread asymptotic phase method (Damburg and Kolosov 1976), based on the Breit-Wigner parameterization for the asymptotic phase shift dependence on scattering energy and the method by Luc-Koenig and Bachelier, who have used a normalization constant [42,48]. Different calculational procedures are used in the Pade and then Borel summation of the divergent Rayleigh-Schrödinger perturbation theory (PT) series (Franceschini et al 1985, Popov et al 1990) and in the sufficiently exact numerical solution of the difference equations following from expansion of the wave function over finite basis (Benassi and Grecchi 1980, Maquet et al 1983, Kolosov 1987, Telnov 1989, Anokhin-Ivanov 1994), complex-scaling method [17-55]. It should be noted that the latter has been extensively used to describe the resonance behavior in different atomic and even molecular systems. Its mathematical foundation is linked with the theory of dilatation analyticity [27,28]. Surely, though the Hamiltonian of an atom in a DC electric field is not a dilatational analytic operator, Reinhardt [44] has performed the numerical experiments on the diagonalization of the complex-scaled Stark Hamiltonian for a hydrogen with a real L basis set. The same method has been used by Cerjan et al. [40] to get new data on the ground and low-excited states of a hydrogen atom in a DC and AC fields. Farrelly and Reinhardt [47] have used the complex coordinate rotation method in combination with numerical integration of the separated equation. Ivanov-Ho [54] have applied the method for the Dirac Hamiltonian. Different applications are reviewed in Refs. [53]. Hehenberger, McIntosh and E. Brändas (1974) [21] have applied the Weyl's theory to the Stark effect in the hydrogen atom. They have shown that one of the interesting features of Weyl's theory is that it requires a complex parameter and complex solutions to the differential equations making it a powerful tool for the treatment of resonance states [21]. Rittby, Elander and Brändas (1981) [25] have applied the Weyl's theory and the complex-rotation method to phenomena associated with a continuum spec-

trum. Brändas and Froelich (1977) [23] have shown that a complex scale transformation of the time-dependent Schrödinger equation leads to a symmetric EE value problem containing both bound states and resonance (complex) EE values as solutions. They have stated the extended virial theorem and developed an original approach to determination of the resonance eigenvalues by means of elementary matrix manipulations. The error estimates for the approximate complex eigenvalues of the dilated Schrödinger operator are derived in Ref. [24], where the calculation data for the resonances of the DC Stark effect in the hydrogen are presented. In the complex-coordinate method a dilation transformation is used to make the resonance EF square integrable. The resonance of nondilation analytic potentials can be obtained numerically by using Simons exterior-scaling procedures within the finite-basis-set approximation [27,28]. The exterior-scaling procedure has been used only with direct numerical integration methods [27-30]. The use of a finite basis set in these calculations will enable one to use numerical techniques developed for bound states in calculating resonance positions and widths for nondilation potentials [27-36]. Rao, Liu and Li (1994) [18]) have studied theoretically the DC strong-field Stark resonances by a complex-scaling plus B-spline approach and shown that the high accuracy is attributed to the good stationarity behavior of eight trajectories with a well-adjusted 8-spline basis. Rao and Li (1995) [19] have also studied the behavior of the resonances of a hydrogen atom in parallel magnetic and electric fields with a complex scaling plus B-spline method too and received a consistent data on the corresponding resonance parameters in dependence upon the ratio of the magnetic-field strength to the electric-field strength. It is worth to remind that the similar approaches have been developed to describe the Zeemane resonances. Namely, for hydrogen atoms in pure magnetic fields, the properties of resonant states were calculated by the complex scaling, the R matrix, the operator PT (OPT) and other methods (look, for example, [4-7]. The generalization of methods to account for the resonance interference, non-H and relativistic effects is still an important problem,

though here a definite progress has been reached too. One should mention such approaches as a model potential method, quantum defect approximation, the OPT, complex scaling plus B-spline method etc [3-19, 64-75]. Regarding the quantum chaos phenomenon in atoms in electromagnetic fields (look, for example, [76-79]) note that this topic should not be considered here. Let us only note that the approach presented below together with the various methods of the theory of chaos in options [79-81] has been effectively used to describe the chaotic behavior

of the hydrogen and non-H atoms in the magnetic and microwave fields.

Here a consistent uniform quantum-mechanical approach to the solution of the non-stationary state problems including the DC strong-field Stark effect and also scattering problem is presented. It allows calculation of complex EE and especially is destined for investigation of the spectral region near the new continuum boundary. The essence of the method is the inclusion of the well known “distorted waves approximation” method in the frame of the formally exact PT. The zero-order Hamiltonian H_0 of this PT possesses only stationary bound and scattering states. To overcome formal difficulties, we define the zero-order Hamiltonian by the set of orthogonal eigenfunctions (EF) and EE without specifying the explicit form of the corresponding zeroth-order potential. To ensure rapid PT convergence, a physically reasonable spectrum (EE and EF) must be chosen as the zero order, similar to the “distorted waves” method [6,56-58]. In a case of the optimal zeroth-order spectrum, the PT smallness parameter is of the order of Γ/A , where Γ and E are the field width and bound energy of the state level examined. The successive PT corrections can be expressed through the matrix elements of the total Hamiltonian calculated between the zeroth-order basis functions. This method is called the OPT. We will define H_0 so that it coincides with the total Hamiltonian H at $\varepsilon \rightarrow 0$ (e is the electric field strength.) Let us emphasize that perturbation in our theory does not coincide with the electric field potential though they disappear simultaneously. We also present a generalization of the OPT for calculation of the DC strong field Stark effect in

the non-H atoms in an electric field [59-61]. The difference between the atomic and Coulomb field is taken into account by introducing the quantum defects on a parabolic basis. The results of calculation of the Stark resonance energies and widths for the H atom are listed and compared with other theoretical and experimental data.

2 Operator perturbation theory for DC strong-field Stark effect

2.1. DC strong –field Stark effect for the hydrogen atom

The Schrödinger equation for the electron function taking into account the uniform electric field and field of the nucleus (Coulomb units are used: for length, 1 unit is \hbar^2/Ze^2m ; for energy 1 unit is mZe^2e^4/\hbar^2) is [6,57]:

$$[-(1 - N/Z) / r + V_m(r) + \varepsilon z - 1/2\Delta - E] \Psi = 0, \quad (1)$$

where E is the electron energy, Z is the nucleus charge, N is the number of electrons in the atomic core (for the hydrogen atom: $Z=1, N=0$), V_m is a model potential (for the hydrogen atom $V_m=0$). Firstly, we only deal with the Coulomb part of the electron- atomic residue interaction. The non-Coulomb part, as well as relativistic effects, can be approximately accounted for next step. The separation of variables in the parabolic coordinates ($\xi = r + z, \eta = r - z, \varphi = \tan^{-1}(y/x)$):

$$\Psi(\varepsilon, h, \varphi) = f(\varepsilon)g(h)(\varepsilon \times h)^{|m|/2} \exp(im\varphi) / (2\pi)^{1/2} \quad (2)$$

transforms it to the system of two equations for the functions f, g :

$$f'' + \frac{|m|+1}{t} f' + [1/2E + (\beta_1 - N/Z)/t - 1/4\varepsilon(t)t] f = 0, \quad (3)$$

$$g'' + \frac{|m|+1}{t} g' + [1/2E + \beta_2 / t + 1/4\varepsilon(t)t] g = 0, \quad (4)$$

coupled through the constraint on the separation constants:

$$\beta_1 + \beta_2 = 1 \quad (5)$$

For the uniform electric field $\varepsilon(t) = \varepsilon$. In principle, the more realistic models can be considered in the framework of our approach. 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 ($\beta = \beta_1$, $E = E_0$):

$$t_2 = \{ [E_0^2 - 4\varepsilon(1-\beta)]^{1/2} - E_0 \} / \varepsilon, \quad (6)$$

$$t_1 = \{ -[E_0^2 - 4\varepsilon(1-\beta)]^{1/2} - E_0 \} / \varepsilon, \quad t_1 < t_2 \quad (7)$$

Here and below t denotes the argument common for the whole equation system. To simplify the calculational procedure, the uniform electric field ε in (3) and (4) should be substituted by the function [57,58]:

$$\varepsilon(t) = \frac{1}{t} \varepsilon \left[(t - \tau) \frac{\tau^4}{\tau^4 + t^4} + \tau \right] \quad (8)$$

with sufficiently large r ($r=1.5t_2$). The function $\varepsilon(t)$ practically coincides with the constant ε in the inner barrier motion region ($t < t_2$) and disappears at $t \gg t_2$. The minimal acceptable value of t introduced in the spatial dependence of the electric field, which does not influence the final results, can be established experimentally. Thus, the final results do not depend on the parameter t (the further calculation has entirely confirmed this fact). Besides the pure technical convenience, the case of an asymptotically disappearing electric field is more realistic from the physical point of view. Now we deal with the asymptotically free (without electric field) motion of the ejected electron along the h -axis. The corresponding effective wavenumber is:

$$k = (E/2 + \varepsilon t/4)^{1/2}. \quad (9)$$

The scattering states energy spectrum now spreads over the range $(-\varepsilon/2, +\infty)$, compared with $(-\infty, +\infty)$ in the uniform field. In contrast to the case of a free atom in scattering states in the presence of the uniform electric field remain quantified at any energy E , i.e. only definite values of β_1 are possible. The latter are de-

termined by the confinement condition for the motion along the h -axis. The same is true in our

case, but only for $E \in \left(-\frac{1}{2}\varepsilon\tau, +\frac{1}{2}\varepsilon\tau\right)$. The motion with larger E is non-quantified, similar to the free atom case.

2.2 Energy and width of the Stark resonance

The total Hamiltonian $H(\zeta, \nu, \varphi)$ does not possess the bound stationary states. According to OPT [6, 56-58]), one has to define the zero order Hamiltonian H_0 , so that its spectrum reproduces qualitatively that of the initial one. In contrast to H , it must have only stationary states. To calculate the width G of the concrete quasistationary state in the lowest PT order one needs only two zeroth-order EF of H_0 : bound state function $\Psi_B(\varepsilon, \eta, \varphi)$ and scattering state function $\Psi_E(\varepsilon, \eta, \varphi)$ with the same EE. We solve a more general problem: a construction of the bound state function along with its complete orthogonal complementary of

scattering functions Ψ_E with $E \in \left(-\frac{1}{2}\varepsilon\tau, +\infty\right)$.

First, one has 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 [65,66]. Following [57], we solve the system (3) and (4) with the total Hamiltonian H under the conditions:

$$f(t) \rightarrow 0 \text{ at } t \rightarrow \infty, \quad (10a)$$

$$ax(\beta, E) / DE = 0 \quad (10b)$$

with

$$x(b, E) = \lim_{t \rightarrow \infty} [g^2(t) + \{g^1(t)/k\}^2] t^{m+1}. \quad (11)$$

The first condition ensures the finiteness of motion along the ζ -axis, the second condition minimizes the asymptotic oscillation amplitude for the function describing the motion along the η -axis. These two conditions quantify the bound energy E and separation constant β_1 . We elaborated a special numerical procedure for this two-dimensional eigenvalue problem. Our procedure deals repeatedly with the solving of the system of the ordinary differential equations (3) and (4) with probe pairs of E, β_1 . The corresponding EF:

$$y_{E_b}(\zeta, \eta, \varphi) = f_{E_b}(\zeta) g_{E_b}(\eta) (\zeta \eta)^{|m|/2} \exp(im\varphi) (2\eta)^{-1/2} \quad (12)$$

Here $f_E(t)$ is the solution of (3) (with the just determined E, β_1) at $t \in (0, \infty)$ and $g_{E_b}(t)$ is the solution of (4) (with the same E, β_1) at $t < t_2$ (inside barrier) and $g(t) = 0$ otherwise. These 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 the quantum numbers n, n_1, n_2, m (principal, parabolic, azimuthal) connected with E, β_1, m by the well known expressions. We preserve the n, n_1, m states classification in the non-zero ε case. The scattering state functions:

$$\Psi_{E_s}(\zeta, \eta, \varphi) = f_{E_s}(z) g_{E_s}(\eta) (\zeta \eta)^{|m|/2} \exp(im\varphi) (2\pi)^{-1/2} \quad (13)$$

must be orthogonal to the above defined bound state function and to each other. In addition, these functions must describe the motion of the ejected electron, i.e. g_{E_s} must satisfy the equation (4) asymptotically. Following the OPT ideology [57], we choose the next form of g_{E_s} :

$$g_{E_s}(t) = g_1(t) - z_2' g_2(t) \quad (14)$$

with f_{E_s} and $g_1(t)$ satisfying the differential equations (3) and (4). The function $g_2(t)$ satisfies the non-homogeneous differential equation, which differs from (4) only by the right-hand term, disappearing at $t \rightarrow \infty$. The total equation system, determining the scattering function, reads

$$f''_{E_s} + \frac{|m|+1}{t} f'_{E_s} + [1/2E' + (\beta_1' - N/Z) / t - 1/4] \cdot \varepsilon(t) f_{E_s} = 0, \quad (15a)$$

$$g_1'' + \frac{|m|+1}{t} g_1' + [1/2E' + \beta_2' / t + 1/4 \varepsilon(t)] g_1 = 0, \quad (15b)$$

$$g_2'' + \frac{|m|+1}{t} g_2' + [1/2E' + \beta_2' / t + 1/4 \varepsilon(t)] g_2 = 2g_{E_b} \quad (15c)$$

($\beta_1' + \beta_2' = 1$). As mentioned above there remains

motion quantification for $A' \subset \left(-\frac{1}{2}\varepsilon\tau, +\frac{1}{2}\varepsilon\tau\right)$.

At the given E' , the only quantum parameter β_1'

is determined by the natural boundary condition:

$f_{E_s} \rightarrow 0$ at $t \rightarrow \infty$. Of course: $\beta_1' = \beta_1, f_{E_s} = f_{E_b}$ at $E' = E$; only this case is needed in the particular problem we deal with here. The coefficient z_2' ensures the orthogonality condition $\langle \Psi_{E_b} | \Psi_{E_s} \rangle = 0$:

$$z_2' = \frac{\iint d\zeta d\eta (\zeta + \eta) f_{E_b}^2(\zeta) g_{E_b}(\eta) g_1(\eta)}{\iint d\zeta d\eta (\zeta + \eta) f_{E_b}^2(\zeta) g_{E_b}(\eta) g_2(\eta)}. \quad (16)$$

One can check that

$$\langle \Psi_{E_s} | \Psi_{E'_s} \rangle = 0 \text{ for } E' \neq E''.$$

The imaginary part of state energy in the lowest PT order is

$$\text{Im}E = \Gamma/2 = \pi |\langle \Psi_{E_b} | H | \Psi_{E_s} \rangle|^2 \quad (17)$$

with the total Hamiltonian H . The state functions Ψ_E and $\Psi_{E'}$ are assumed to be normalized to 1 and by the $\delta(k - k')$ condition, accordingly. The action of H on Ψ_E is defined unambiguously by (15):

$$(H - E') \Psi_s = 2|m| (\zeta \cdot \eta^2) \cdot f_{E_s}(\zeta) g_{E_b}(\eta) z_2' \exp(im\varphi) / [(2\pi)^{1/2} (\zeta + \eta)], \quad (18)$$

$$\langle \Psi_{E_b} | H | \Psi_{E_s} \rangle = \iint d\zeta d\eta (\zeta \eta)^{|m|} \eta f_{E_b}^2(\zeta) f_{E_s}^2(\zeta) g_{E_b}(\eta) z_2'.$$

The matrix elements $\langle \Psi_E | H | \Psi_{E_s} \rangle$ entering the high-order PT corrections can be determined in the same way. All the two-dimensional integrals in (16)-(18) and the normalization coefficients can be expressed through the next set of one-dimensional integrals:

$$\begin{aligned} I_2 &= \int dt f_b^2(t) t^{|m|+1}, \\ I_3 &= \int dt g_b(t) g_1(t) t^{|m|}, \\ I_4 &= \int dt g_b(t) g_1(t) t^{|m|+1}, \\ I_5 &= \int dt g_b(t) g_2(t) t^{|m|}, \\ I_6 &= \int dt g_b(t) g_2(t) t^{|m|+1}, \\ I_7 &= \int dt g_b^2(t) t^{|m|}, \\ I_8 &= \int dt g_b^2(t) t^{|m|+1}, \end{aligned} \quad (19)$$

calculated with the arbitrary normalized functions $f_{E_b}, g_{E_b}, f_2, g_2$ and $f_1 = f_{E_b}, g_1 = g_{E_b}$. In

this notation

$$\Gamma = 32\pi z_2^2 N_s^2 I_1^2 I_8^2 / [I_2 I_7 + I_1 I_8],$$

$$z_2 = [I_1 I_4 + I_2 I_3] / [I_1 I_6 + I_2 I_5] \quad (20)$$

with

$$N_s^2 = \lim_{t \rightarrow \infty} X(t) / \{2\pi\eta^{2|m|+1} [g_s^2(\eta)X^2(t) + g_s'^2(\eta)]\}$$

$$X(t) = \{E/2 + (\beta - N/Z)/t - E t/4\}^{1/2} \quad (21)$$

Remember that arbitrary normalized state functions are assumed in (20) and (21). The whole calculational procedure at known resonance energy E and separation parameter β_1 has been reduced to the solution of one system of the ordinary differential equations. This master system includes the differential equations for the state functions f_{Eb} , g_{Eb} , f_{Es} , g_{Es} , as well as the equations for the integrals $I_1 - I_8$. Thus, our calculational procedure is one-dimensional. The procedure is sufficiently simple and realized as the numerical code with using the fourth-order Runge–Kutta method of solving the differential equations (the atomic code “Superatom-ISAN-Stark”).

3 Calculation results and discussion

The calculation results for the Stark resonances energies and widths of the ground state hydrogen atom in the DC electric field with the strength $\varepsilon=0.04, 0.08, 0.10, 0.80$ a.u. are presented in table 1 and 2. The comparison with earlier similar results, obtained within the generalized WKB approximation, summation of divergent PT series, the numerical solution of the differential equations following from expansion of the wave function over finite basis, a complex scaling plus B-spline calculation [15-51] shows quite acceptable agreement. The calculation results of the Stark resonances parameters for the excited state H atom ($n=2,5,15$) for different strength values are listed in table 3. The comparison with earlier similar results, obtained within the summation of divergent PT series, the numerical solution of the differential equations with using the finite basis expansion of the wave function again shows acceptable agreement.

Table 1. Energies, widths (a.u.)of Stark resonances of ground state H atom ($\varepsilon=0.04, 0.08$ a.u.). Notation: (a1) Mendelson [15], (a2) Alexander [17], (b1) Hehenberger- McIntosh-Brändas [21], (b2) Brändas-Froelich [23], (c) Benassi-Grecchi [46], (d) Cerjan et al. [40], (e) Farrelly-Reinhardt [47], (f) Franceschini-Greechi-Silverstone [45], (g) Reinhardt [43], (h) Maquet-Chu-Reinhardt [41], (i) Kolosov [48], (j) Damburg-Kolosov [42], (k) Anokhin-Ivanov [51], (l) Ivanov-Ho (relativistic and non-relativistic results respectively) [54], (m) Rao- Liu-Li [18], (n) the OPT method (our data), (o) – Filho et al [49].

ε	Method	E_r , a.u.	$\Gamma/2$, a.u.
0.04	a1	-0.5038	-
	a2	-0.5038	0.2×10^{-5}
	b1	-0.5037714	0.195×10^{-5}
	b2	-0.5037715	0.191×10^{-5}
	c	-0.5037716	0.1946×10^{-5}
	f	-0.5037716	0.1946×10^{-5}
	j	-0.5037716	0.195×10^{-5}
	k	-0.5038	0.248×10^{-5}
	l	-0.5037780 -05037716	0.205×10^{-5} 0.195×10^{-5}
	m	-05037716	0.1946×10^{-5}
n	-05037714	0.1945×10^{-5}	
o	-0503752	-	
0.08	a1	-0.5193	-
	a2	-0.5175	0.230×10^{-2}
	b1	-0.51756	0.227×10^{-2}
	c	-0.51756	0.2270×10^{-2}
	f	-0.51756	0.2270×10^{-2}
	g	-0.51756	0.2269×10^{-2}
	h	-0.51756	0.2270×10^{-2}
	j	-0.51749	0.2255×10^{-2}
	k	-0.5176	0.220×10^{-2}
	m	-0.51756	0.2270×10^{-2}
n	-0.51757	0.2270×10^{-2}	
o	-0.51745	-	

Table 2. Energies and widths of the 1s H atom Stark resonances ($\varepsilon=0.10,0.8$ a.u.); Notation: (a1) Mendelson [15], (a2) Alexander [17], (b1) Hehenberger-McIntosh-Brändas [21], (b2) Brändas-Froelich [23], (c) Benassi-Grecchi [46], (d) Cerjan et al. [40], (e) Farrelly-Reinhardt [47], (f) Franceschini-Grecchi-Silverstone [45], (g) Reinhardt [43], (h) Maquet-Chu-Reinhardt [41], (i) Kolosov [48], (j) Damburg-Kolosov [42], (k) Anokhin- Ivanov [51], (l) Ivanov-Ho [54], (m) Rao, Liu and Li [18], (n) OPT method, (o) – Filho et al [49], (p)- Popov et al [65,66].

ε	Method	E_r , a.u.	$\Gamma/2$, a.u.
0.10	a1	-0.556	-
	a2	-0.527	0.7500×10^{-2}
	b1	-0.52743	0.7250×10^{-2}
	b2	-0.52742	0.7270×10^{-2}
	c	-0.527418	0.7269×10^{-2}
	d	-0.527417	0.7270×10^{-2}
	f	-0.527418	0.7269×10^{-2}
	g	-0.527425	0.7271×10^{-2}
	h	-0.527418	0.7269×10^{-2}
	i	-0.527418	0.7269×10^{-2}
	j	-0.526905	0.7170×10^{-2}
	l	-0.527423	0.7268×10^{-2}
		-0.527418	0.7269×10^{-2}
	m	-0.527418	0.7269×10^{-2}
	n	-0.527419	0.7269×10^{-2}
		o	-0.531090
	p	-0.5274	0.727×10^{-2}
0.80	e	-0.6304	0.5023
	i	-0.630415	0.50232
	m	-0.630415	0.50232
	n	-0.630416	0.50232

It is important to compare the theoretical values of the resonance energy and width for the H atom in the field $\varepsilon = 16.8$ kV/cm with experimental data [4]. There is quite good agreement between theory and experiment. Note that our results are obtained in the first PT order, i.e. already the first PT order provides the physically reasonable results. Naturally its accuracy can be increased by an account of the next PT order. The range of validity of the proposed method which

uses the Fermi golden rule is quite wide and it is not restricted to resonances lying far from the continuum boundary.

Table 3. The energies and widths of the Stark resonances of the hydrogen atom ($n=2,5$). Notation: a, OPT calculation; b, Damburg and Kolosov (1976); c, Kolosov (1987); d, Benassi and Grecchi (1980); e, Telnov (1989); f, Popov et al (1990); E_x – experimental data (from Refs. [4, 42, 46,48,57,58,65,66]).

$(n \ n_1 \ n_2 \ m)$	ε , a.u.	Method	E_r , a.u.	Γ , a.u.
2 0 1 0	0,005	a	0.1426	$0.102 \cdot 10^{-3}$
		c	0.1426	$0.106 \cdot 10^{-3}$
		e	0.1426	$0.106 \cdot 10^{-3}$
	0,01	a	0.1661	$0.108 \cdot 10^{-1}$
		c	0.1661	$0.109 \cdot 10^{-1}$
		d	0.1661	$0.109 \cdot 10^{-1}$
2 0 0 1	0.005	a	0.1272	$0.267 \cdot 10^{-4}$
		c	0.1272	$0.262 \cdot 10^{-4}$
		e	0.1272	$0.262 \cdot 10^{-4}$
	0.01	a	0.1345	$0.637 \cdot 10^{-2}$
		c	0.1345	$0.628 \cdot 10^{-2}$
		e	0.1345	$0.628 \cdot 10^{-1}$
5 2 2 0	$1.8 \cdot 10^{-4}$	a	0.2062	$0.278 \cdot 10^{-5}$
		b	0,2062	$0.228 \cdot 10^{-5}$
		f	0.2062	$0.228 \cdot 10^{-5}$
		f	0.2062	$0.222 \cdot 10^{-5}$
15 10 4 0	$3.27 \cdot 10^{-6}$	a	$1.9098 \cdot 10^{-3}$	$2.782 \cdot 10^{-7}$
		f	$1.9095 \cdot 10^{-3}$	$2.278 \cdot 10^{-7}$
		E_x	$1.91 \cdot 10^{-3}$	$2.92 \cdot 10^{-7}$

4. Conclusions

In this paper we present the bases of a new uniform quantum-mechanical approach to the solution of the non-stationary state problems including the DC strong-field Stark effect and also scattering problem. New OPT method allows sufficiently exact calculating the complex EE and resonance widths and especially is destined for investigation of the spectral region of an atom near the new continuum boundary in a strong field. The essence of the method is the inclusion of the well known “distorted waves approximation” in

the frame of the formally exact PT. The results of the calculation of the Stark resonance energies and widths for the hydrogen atom are presented and in a physically reasonable agreement with the best results of the alternative theoretical methods and experiment. It is noted that the zeroth model approximation, including the potential of a strong external electric field, can be implemented into the general formalism of the formally exact PT for many-electron atom [6,12,59-63,71-75]. The range of validity of the presented method which uses the Fermi golden rule is sufficiently wide and it is not restricted to resonances lying far from the continuum boundary. Let us conclude that the OPT method has been also successfully applied to correct description of the resonances of the Zeeman effect in a strong magnetic field, crossed electric and magnetic fields, the resonances in molecular systems, as well as descriptions of resonant states in nuclear systems such as the resonances of the compound nucleus and the resonances arising from the collision of heavy ions (nuclei), accompanied by electron-positron pairs production (look Refs. [6,79,82-90]).

References

1. J. Stark, *Ann.Phys.* **43**, 965 (1914).
2. H. A. Bethe and E.E. Salpeter, *Quantum mechanics of One- and Two-Electron Atoms* (Springer, Berlin, 1957).
3. L. D. Landau and E. M. Lifshitz, *Quantum Mechanics* (Pergamon, Oxford, 1977).
4. R. F. Stebbings and F. B. Dunning (ed), *Rydberg States of Atoms and Molecules* (Cambridge Univ. Press, N.-Y., 1983).
5. M.N. Nayfeh and C.W. Clark (ed), *Atomic Excitation and Recombination in External Fields* (NBS, Gaithersburg, 1984).
6. A. V. Glushkov, *Atom in an Electromagnetic Field* (KNT, Kiev, 2005), pp.1-450.
7. V. S. Lisitsa, *Phys.-Uspekhi* **153**, 369 (1987).
8. L. N. Ivanov and V. S. Letokhov, *Quantum Electron.* **2**, 585 (1975).
9. L. N. Ivanov and E.P.Ivanova, *Atom. Data Nucl. Data Tabl.* **24**, 95 (1979).
10. A. V. Glushkov and L. N. Ivanov, *Phys. Lett. A* **170**, 33 (1992).
11. E. P. Ivanova and I. P. Grant, *J. Phys.B: At. Mol. Opt. Phys.* **31**, 2871 (1998).
12. A. V. Glushkov, in: *Advances in the Theory of Quantum Systems in Chemistry and Physics. Series: Frontiers in Theoretical Physics and Chemistry*, vol.26, ed. by K.Nishikawa, J. Maruani, E.Brändas, G.Delgado-Barrio, P.Piecuch (Berlin, Springer, 2012), pp.231-254.
13. N. B. Delone and M.V. Fedorov, *Phys.-Uspekhi.* **158**, 215 (1989).
14. A. J. F. Siegert, *Phys.Rev.* **56**, 750 (1939).
15. L. B. Mendelson, *Phys. Rev.* **176**, 90 (1968).
16. A. D. Dolgov and A.V. Turbiner, *Phys. Lett. A* **77**, 15 (1977).
17. M. H. Alexander, *Phys. Rev.* **178**, 34 (1969).
18. J. Rao, W. Liu and B. Li, *Phys. Rev. A* **50**, 1916 (1994).
19. J. Rao and B. Li, *Phys. Rev. A* **51**, 4526 (1995).
20. H.-Y. Meng, Y.-X. Zhang, S. Kang, T.-Y. Shi and M.-S. Zhan *J. Phys. B: At. Mol. Opt. Phys.* **41**, 155003 (2008).
21. M. Hehenberger, H.V. McIntosh and E. Brändas, *Phys. Rev. A* **10**, 1494 (1974).
22. M. Hehenberger, H. V. McIntosh and E. Brändas, *Phys. Rev. A* **12**, 1 (1975).
23. E. Brändas and P. Froelich, *Phys. Rev. A* **16**, 2207 (1977).
24. E. Brändas, M. Hehenberger and H. V. McIntosh, *Int. J.Quant.Chem.* **9**, 103 (1975).
25. M. Rittby, N. Elander and E. Brändas, *Phys. Rev. A* **24**, 1636 (1981).
26. P. Froelich, E. R. Davidson, E. Brändas, *Phys. Rev. A* **28**, 2641 (1983).
27. N. Lipkin, N. Moiseyev and E. Brändas, *Phys. Rev. A* **40**, 549 (1989).
28. M. Rittby, N. Elander and E. Brändas, *Int. J.Quant.Chem.* **23**, 865 (1983).
29. B. Simon, *Phys.Lett. A* **71**, 211 (1979).
30. C.A. Nicolaidis and D.R. Beck, *Phys. Lett. A* **65**, 11 (1978).
31. E. Brändas, P. Froelich, C. H. Obcemea,

- N. Elander, M. Rittby, *Phys. Rev. A* **26**, 3656 (1982).
32. E. Engdahl, E. Brändas, M. Rittby, N. Elander, *J. Math. Phys.* **27**, 2629 (1986)
 33. E. Engdahl, E. Brändas, M. Rittby and N. Elander, *Phys. Rev. A* **37**, 3777 (1988).
 34. Resonances. The Unifying Route Towards the Formulation of Dynamical Processes - Foundations and Applications in Nuclear, Atomic and Molecular Physics, Series: Lecture Notes in Physics, vol. **325**, ed. by E. Brändas, N. Elander (Springer, Berlin, 1989), pp.1-564.
 35. A. Scrinzi and N. Elander, *J. Chem. Phys.* **98**, 3866 (1993)
 36. V. N. Ostrovsky and N. Elander, *Phys. Rev. A* **71**, 052707 (2005)
 37. J. M. Sigal, *Commun. Math. Phys.* **119**, 287 (1988).
 38. I.W. Herbst and B. Simon, *Phys. Rev. Lett.* **41**, 67 (1978).
 39. H. J. Silverstone, B. G. Adams, J. Cizek and P.Otto, *Phys. Rev. Lett.* **43**, 1498 (1979).
 40. C. Cerjan, R. Hedges, C. Holt, W. P. Reinhardt, K. Scheibner and J. J. Wendoloski, *Int.J.Quant.Chem.* **14**, 393 (1978).
 41. Maquet, S. I. Chu and W. P. Reinhardt, *Phys. Rev. A* **27**, 2946 (1983).
 42. R. J. Damburg. and V.V. Kolosov, *J. Phys.B: At. Mol. Phys.* **9**, 3149 (1976).
 43. E. Luc-Koenig and A. Bachelier, *J. Phys.B: At. Mol. Phys.* **13**, 1743 (1980).
 44. W. P. Reinhardt, *Int.J.Quant.Chem.* **21**, 133 (1982).
 45. V. Franceschini, V. Grecchi and H.J. Silverstone, *Phys. Rev. A* **32**, 1338 (1985).
 46. L. Benassi and V. Grecchi, *J. Phys. B: At. Mol. Phys.* **13**, 911-24 (1980).
 47. D. Farrelly and W.P. Reinhardt, *J. Phys. B: At. Mol. Phys.* **16**, 2103 (1983).
 48. V. V. Kolosov, *J. Phys. B: At. Mol. Phys.* **20**, 2359 (1987).
 49. Filho, A. Fonseca, H. Nazareno and P. Guimarães, *Phys. Rev. A* **42**, 4008 (1990).
 50. V. D. Kondratovich and V. N. Ostrovsky, *J. Phys. B: At. Mol. Phys.* **17**, 2011 (1984).
 51. S. B. Anokhin and M. V. Ivanov, *Opt. Spectr.* **59**, 499 (1984).
 52. D. A. Telnov, *J. Phys. B: At.Mol. Opt. Phys.* **22**, 1399-403 (1989).
 53. Y.-K. Ho, *Phys.Rep.* **99**, 3 (1983).
 54. I. A. Ivanov, and Y.-K. Ho, *Phys.Rev. A* **69**, 023407 (2004).
 55. R. González-Férez and W. Schweizer, in *Quantum Systems in Chemistry and Physics*, Series: Progress in Theoretical Chemistry and Physics, vol. **2/3**, ed. by A. Hernández-Laguna, J. Maruani, R. McWeeny, S.Wilson (Springer, Berlin, 2000), p. 17.
 56. A. V. Glushkov and L. N. Ivanov, *Proc. of 3rd Symposium on Atomic Spectroscopy (Moscow-Chernogolovka, 1992)*.
 57. A. V. Glushkov and L. N. Ivanov, *J. Phys.B: At. Mol. Phys.* **26**, L379 (1993).
 58. A. V. Glushkov, S. V. Malinovskaya, S. V. Ambrosov, I. M. Shpinareva, O. V. Troitskaya, *J. Techn. Phys.* **38**, 215 (1997).
 59. A. V. Glushkov, S. V. Ambrosov, A. V. Ignatenko, D.A. Korchevsky, *Int.J.Quant. Chem.* **99**, 936 (2004).
 60. A. V. Glushkov and A. V. Loboda, *J. Appl.Spectr. (Springer)* **74**, 305 (2007).
 61. A. V. Glushkov, O. Yu. Khetselius, A. V. Loboda, A.A. Svinarenko, in *Frontiers in Quantum Systems in Chemistry and Physics*, Series: Progress in Theoretical Chemistry and Physics, vol. **18**, ed. by S. Wilson, P.J. Grout., J. Maruani, G. Delgado-Barrio, P. Piecuch (Springer, Berlin, 2008), pp.523-588;
 62. A. V. Glushkov, O. Khetselius, S. Malinovskaya, *Europ.Phys. Journ.* **T160**, 195 (2008).
 63. A. V. Glushkov, O. Yu. Khetselius, A. A. Svinarenko and G.P.Prepelitsa, in: *Coherence and Ultrashort Pulsed Emission*, ed. F.J. Duarte. (Intech, Vienna, 2011), pp.159-186.
 64. M. L. Zimmerman, M.G. Littman, M.M. Kash, D. Kleppner, *Phys. Rev.* **A20**, 2251 (1979).
 65. D.A. Harmin, *Phys.Rev. A* **26**, 2656 (1982).
 66. V. Popov, V. Mur, A. Sergeev and

- V. Weinberg, *Phys.Lett.A* **149**, 418, 425 (1990).
67. M. Grutter, O.Zehnder, T.Softley, F.Merkt, *J.Phys.B: At. Mol. Opt. Phys.* **41**, 115001 (2008).
 68. E. Stambulchik and Y. Maron, *J. Phys. B: At. Mol. Opt. Phys.* **41**, 095703 (2008).
 69. F. B. Dunning, J. J. Mestayer, C. O. Reinhold, S. Yoshida and J Burgdörfer, *J. Phys. B: At. Mol. Opt. Phys.* **42**, 022001 (2009).
 70. H. C. Bryant, D. A. Clark, K. B. Butterfield et al, *Phys.Rev.A* **27**, 2889 (1983).
 71. A. V. Glushkov, S. Ambrosov, O. Yu. Khetselius, A. V. Loboda, E. Gurnitskaya, in: *Recent Advances in Theoretical Physics and Chemistry Systems, Series: Progress in Theoretical Chemistry and Physics*, vol. 15, ed. by J.-P. Julien, J. Maruani, D. Mayou, S. Wilson, G. Delgado-Barrio (Springer, Berlin, 2006), pp. 285-300.
 72. Yu. Khetselius, *J. Phys.: Conf.Ser.* **397**, 012012 (2012); *Int.J.Quant.Chem.* **109**, 3330 (2009).
 73. O. Yu. Khetselius, T. Florko, A. Svinarenko and T. Tkach, *Phys.Scr.* **T153**, 01437 (2013).
 74. E. P. Ivanova, L. N. Ivanov, A. V. Glushkov and A.E. Kramida, *Phys. Scr.* **32**, 512 (1985).
 75. E. P. Ivanova and A. V. Glushkov, *J.Quant. Spectr. Rad. Tr.* **36**, 127 (1986).
 76. F. Benvenuto, G. Casati and D.L. Shepelyansky, *Z.Phys.B.* **94**, 481 (1994).
 77. A. Buchleitner and D. Delande, *Phys. Rev.A.* **55**, 1585 (1997).
 78. T.F. Gallagher, M. Noel and M.W. Griffith, *Phys. Rev. A.* **62**, 063401 (2000).
 79. A. V. Glushkov and S. V. Ambrosov, *J. Techn. Phys.* **37**, 347 (1996).
 80. A.V. Glushkov, V. Khokhlov and I. Tsenenko, *Nonlin. Proc. Geophys.* **11**, 285 (2004).
 81. A. V. Glushkov, V. Khokhlov, N. Loboda and Yu. Bunyakova, *Atm.Env.* **42**, 7284 (2008).
 82. A. V. Glushkov, O. Yu. Khetselius, S. V. Malinovskaya, *Molec.Phys.* **106**, 1257 (2008).
 83. A. V. Glushkov, V. D. Rusov, S. V. Ambrosov, A. V. Loboda, in *New Projects and New Lines of Research in Nuclear Physics*, ed. by G. Fazio, F. Hanappe (World Sci., Singapore, 2003), pp. 126-142.
 84. A. V. Glushkov, in: *Low Energy Antiproton Physics*, vol. **796**, ed. by D. Grzonka, R. Czyzykiewicz, W. Oelert, T. Rozek and P. Winter (AIP, N.-Y., 2005), pp. 206-210.
 85. A. V. Glushkov, in *Meson-Nucleon Physics and the Structure of the Nucleon*, vol. **2**, ed. by S. Krewald, H. Machner (IKP, Juelich, Germany), SLAC eConf C070910 (Menlo Park, CA, USA, 2007), pp.111-117.
 86. A. V. Glushkov, O. Yu. Khetselius, A. V. Loboda and S.V. Malinovskaya, in *Meson-Nucleon Physics and the Structure of the Nucleon*, vol. **2**, ed. by S. Krewald, H. Machner (IKP, Juelich, Germany), SLAC eConf C070910 (Menlo Park, CA, USA, 2007), pp.118-122.
 87. A. V. Glushkov, O. Yu. Khetselius, L. Lovett, E. P. Gurnitskaya, Yu. V. Dubrovskaya, A. V. Loboda, *Int.J. Mod. Phys. A: Particles and Fields, Nucl. Phys.* **24**, 611 (2009).
 88. A. V. Glushkov O. Yu. Khetselius, L. Lovett, in: *Advances in the Theory of Atomic and Molecular Systems: Dynamics, Spectroscopy, Clusters, and Nanostructures. Series: Progress in Theoretical Chemistry and Physics*, vol. **20**, ed. by P.Piecuch, J. Maruani, G. Delgado-Barrio and S. Wilson (Springer, Berlin, 2010), pp.125-151.
 89. A. V. Glushkov, O. Yu. Khetselius, A. A. Svinarenko, in: *Advances in the Theory of Quantum Systems in Chemistry and Physics. Series: Progress in Theoretical Chemistry and Physics*, vol. **22**, ed. by P. Hoggan, E. Brändas, J. Maruani, G. Delgado-Barrio and P. Piecuch (Springer, Berlin, 2012), pp.51-70.
 90. A. V. Glushkov, *Relativistic Quantum Theory. Quantum Mechanics of Atomic Systems* (Astroprint, Odessa, 2008), pp.1-704.

The article is received in editorial 21.05.2013

UDC 539.184

A. V. Glushkov

OPERATOR PERTURBATION THEORY TO HYDROGEN ATOM IN A STRONG DC ELECTRIC FIELD

Abstract.

A consistent uniform quantum approach to the solution of the non-stationary state problems including the DC (Direct Current) strong-field Stark effect and also scattering problem is presented. It is based on the operator form of the perturbation theory for the Schrödinger equation. The method allows calculating the resonance complex energies and widths plus a complete orthogonal complementary of the scattering state functions. The calculation results of the Stark resonance energies and widths for the hydrogen atom are presented and compared with other theoretical data.

Key words: Stark effect, hydrogen atom, DC electric field, operator perturbation theory

УДК 539.184

A. B. Глушков

ОПЕРАТОРНАЯ ТЕОРИЯ ВОЗМУЩЕНИЙ ДЛЯ ОПИСАНИЯ АТОМА ВОДОРОДА В ПОСТОЯННОМ ЭЛЕКТРИЧЕСКОМ ПОЛЕ

Резюме.

Представлен новый, последовательный квантовый подход к решению проблемы нестационарных состояний, включая эффект Штарка для сильных полей, а также задачи рассеяния. Подход основан на операторной теории возмущений для уравнения Шредингера. Метод позволяет рассчитать комплексные энергии и ширины резонансов, а также полный ортогональный набор функций состояний рассеяния. Приведены результаты расчета энергий и ширин штарковских резонансов для атома водорода и проведено сравнение с другими теоретическими данными.

Ключевые слова: эффект Штарка, атом водорода, электрическое поле, операторная теория возмущений

УДК 539.184

O. B. Глушков

ОПЕРАТОРНА ТЕОРІЯ ЗБУРЕНЬ ДЛЯ ОПИСУ АТОМУ ВОДНЮ У СТАЛОМУ ЕЛЕКТРИЧНОМУ ПОЛІ

Резюме.

Представлено новий послідовний квантовий підхід до вирішення проблеми нестационарних станів, включаючи ефект Штарка для сильних полів, а також задачі розсіювання. Підхід заснований на операторній теорії збурень для рівняння Шредингера. Метод дозволяє розрахувати комплексні енергії та ширини резонансів плюс повний ортогональний набір функцій станів розсіювання. Приведені результати розрахунку енергій та ширин штарківських резонансів для