Modified operator perturbation theory computational approach to atomic systems in a DC electric field: Stark resonances

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Abstract. New computational realization of the modified operator perturbation theory method to computing the Stark resonances energies and widths for the non-hydrogenic (non-H) atomic systems in a DC electric field is presented. The method is based on the operator form of the perturbation theory of the Schrödinger equation for the non-H atomic systems and includes the physically reasonable distorted-waves approximation in the frame of the formally exact quantum-mechanical procedure. The Stark resonances energies and widths in the lithium atom are calculated and compared with results of calculations on the basis of the method of complex eigenvalue Schrödinger equation by Themelis-Nicolaides, the complex absorbing potential method by Sahoo-Ho and the B-spline-based coordinate rotation method approach by Hui-Yan Meng et al.

1. Introduction
The Stark effect 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]. At last years it attracts a great interest especially in the multielectron atoms that is stimulated by a whole range of interesting phenomena to be studied such as quasi-discrete state mixing, a zoo of Landau- Zener anticrossings, autoionization in the multielectron atoms, the effects of potential barriers (shape resonances), new kinds of resonances above threshold etc [11-56]. An external electric field shifts and broadens the bound state atomic levels. The standard quantum-mechanical approach relates the 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 (see review in Ref. [58]) are introduced in Stebbings and Dunning, Kondratovich and Ostrovsky, Popov et al; Ivanov-Letokhov [34,35] have fulfilled the first estimations of the effectiveness of the selective ionization of the Rydberg atom using a DC electric and laser fields within the quasiclassical model. Different calculational procedures are used in the Pade and then Borel summation of the divergent Rayleigh-Schrödinger perturbation theory.
the complex coordinate method to the differential equations making it a powerful tool for the treatment of resonance states. Rittby, Elander and Brändas [12] have applied the Weyl’s theory and the complex-rotation method to phenomena associated with a continuum spectrum. Brändas and Froelich 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. It is worth to note that application of the complex coordinate method to a resonance problem has been justified in [20-23]. Themelis and Nicolaides [41-44] adopted an \textit{ab initio} theory to compute the complex energy of multielectron atomic states. Their approach is based on the state-specific construction of a non-Hermitian matrix according to the form of the decaying-state EF which emerges from the complex eigenvalue Schrödinger equation (CESE) theory. Sahoo and Ho [45,46] carried out the calculation the Stark resonances energies and widths in the lithium atom on the base of the complex absorbing potential (CAP) method. Jianguo Rao et al and Hui-Yan Meng et al [38-40] have presented the B-spline-based coordinate rotation method plus the model potential approach and applied it to investigate the complex energies of low-lying resonances of the hydrogen and lithium atoms in an electric field. In Refs.[56-58] it has been presented 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. It is based on the operator form of the perturbation theory (OPT) for the Schrödinger equation.

In this work we present new computational realization of the modified OPT method for the non-H atomic systems and apply it to studying the Stark resonances parameters for the lithium atom in a DC electric field. The Stark resonances parameters energies and widths are calculated and compared with the data of calculations on the basis of the alternative sophisticated complex eigenvalue approaches [40,42,45].

2. Modified operator perturbation theory approach to multielectron atom in an electric field

As usually [56,57], 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 \(h^2/Ze^2m\); for energy 1 unit is \(mZ^2e^2/h^2\)) is:

\[
\left(-\left(1 - N/Z\right)/r + V_m(t) + \varepsilon z - 1/2\Delta - E\right)\psi = 0, \tag{1}
\]

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 that describes interaction with the electron shells for multi-electron atom (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 (\(\xi = r + z, \eta = r - z, \varphi = \tan^{-1}(y/x)\))

\[
\psi(\xi, \eta, \varphi) = f(\xi) g(\eta) (\xi^2 + \eta^2)^{1/4} \exp(i\varphi)/(2\pi)^{1/2} \tag{2}
\]

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

\[
f'' + \left|\frac{n}{t}\right| f' + \left[1/2E + (\beta_l - N/Z)/t - 1/4\varepsilon(t)t\right] f = 0, \tag{3}
\]
coupled through the constraint on the separation constants:

\[
\beta_1 + \beta_2 = 1
\]  

(5)

Let us underline that here and below variable \( t \) denotes the argument common for the whole differential equations system (4). For the uniform electric field \( \varepsilon(t) = \varepsilon \). Potential energy in equation (4) has the barrier. Two turning points for the classical motion along the \( \eta \) axis, \( t_1 \) and \( t_2 \), at a given energy \( E \) are the solutions of the quadratic equation (\( \beta = \beta_1, E = E_0 \)):

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

(6)

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

(7)

To simplify the calculational procedure, the uniform electric field \( \varepsilon \) in (3) and (4) should be substituted by the function [56]:

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

(8)

with sufficiently large \( \tau (\tau = 1.5 t_2) \). The motivation of a choice of the \( \varepsilon(t) \) and some physical features of electron motion along the \( \eta \)-axis are presented in Refs. [56-58]. Here we only underline that the function \( \varepsilon(t) \) practically coincides with the constant \( \varepsilon \) in the inner barrier motion region, i.e. \( t < t_2 \) and disappears at \( t > t_2 \). It is important that the final results do not depend on the parameter \( \tau \). It is carefully checked in the numerical calculation. The scattering states energy spectrum now spreads over the range \((-\varepsilon_1/2, +\infty)\), 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 \( \beta_1 \) are possible. The latter are determined by the confinement condition for the motion along the \( \eta \)-axis. The same is true in our case, but only for \( E < \left(-\frac{1}{2} \varepsilon_1 \eta, +\infty\right)\). Ultimately, such a procedure provides construction of realistic functions of the bound and scattering states. In a certain sense, this completely corresponds to the advantages of the distorted-wave approximation known in scattering theory [61,62].

The total Hamiltonian \( H (\varepsilon, \nu, \varphi) \) does not possess the bound stationary states. According to OPT [37,40], one has to define the zero order Hamiltonian \( H_0 \), so that its spectrum reproduces qualitatively that of the initial one. To calculate the width \( \Gamma \) of the concrete quasistationary state in the lowest PT order one needs only two zeroth–order EF of \( H_0 \); bound state function \( \Psi_{e_b}(\varepsilon, \eta, \varphi) \) and scattering state function \( \Psi_{e_s}(\varepsilon, \eta, \varphi) \) with the same EE. It can be solved a more general problem: a construction of the bound state function along with its complete orthogonal complementary of scattering functions \( \Psi_{e} \) with \( E < \left(-\frac{1}{2} \varepsilon_1 \eta, +\infty\right) \). 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 [2]. The system (3) and (4) with the total Hamiltonian \( H \) is solved under the conditions:
f(t) → 0 at t → ∞ ,

\( \bar{c}(\beta, E) / \partial E = 0 \)

with

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

These two conditions quantify the bound energy \( E \) and separation constant \( \beta_i \). Further one should solve the system of the ordinary differential equations (3) and (4) with probe pairs of \( E, \beta_i \). The corresponding EF:

\[
\psi_{E_1}(\zeta, \eta, \varphi) = f_{E_1}(\zeta) \ g_{E_1}(\eta)(\zeta \eta)^{|m/2|} \ \exp (im\varphi)(2\pi)^{-1/2},
\]

where \( f_{E_1}(t) \) is the solution of (3) (with the just determined \( E, \beta_i \) at \( t < t_2 \)) and \( g_{E_1}(t) \) is the solution of (4)(with the same \( E, \beta_i \) at \( t < t_2 \) (inside barrier) and \( g(t) = 0 \) otherwise.

These bound state EE, eigenvalue \( \beta_i \) and EF for the zero-order Hamiltonian \( H_0 \) coincide with those for the total Hamiltonian \( H \) at \( \varepsilon \to 0 \), where all the states can be classified due to the quantum numbers \( n, n_1, n_2, m \) (principal, parabolic, azimuthal) connected with \( E, \beta_i, m \) by the well-known expressions. The scattering state functions:

\[
\psi_{E_1}(\zeta, \eta, \varphi) = f_{E_1}(\zeta) \ g_{E_1}(\eta)(\zeta \eta)^{|m/2|} \ \exp (im\varphi)(2\pi)^{-1/2}
\]

is 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. \( g_{E_1} \) must satisfy the equation (4) asymptotically. Following the OPT ideology [56], we choose the next form of \( g_{E_1} \):

\[
g_{E_1}(t) = g_1(t) - z \ g_2(t)
\]

with \( f_{E_1} \) 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 \( t \to \infty \). The total equation system, determining the scattering function, reads

\[
f''_{E_1} + \left| m \right| + 1 t f'_{E_1} + \left( 1/2E' + (\beta_1^2 - N/Z) / t - 1/4 \varepsilon(t) \right) f_{E_1} = 0,
\]

\[
g''_1 + \left| m \right| + 1 t g'_1 + \left( 1/2E' + \beta_1^2 / t + 1/4 \varepsilon(t) \right) g_1 = 0,
\]

\[
g''_2 + \left| m \right| + 1 t g'_2 + \left( 1/2E' + \beta_2^2 / t + 1/4 \varepsilon(t) \right) g_2 = 2g_{E_1},
\]

( \( \beta_1^2 + \beta_2^2 = 1 \)). At the given \( E' \), the only quantum parameter \( \beta_1 \) is determined by the natural boundary condition: \( f_{E_1} \to 0 \) at \( t \to \infty \). Of course: \( \beta_1^2 = \beta_0^2 \); \( f_{E_2} = f_{E_0} \) at \( E' = E \); only this case is needed in the particular problem we deal with here. The coefficient \( z \) ensures the orthogonality condition:

\[
\langle \Psi_{E_0} | \Psi_{E_1} \rangle = 0.
\]
The imaginary part of state energy in the lowest PT order is as follows:

$$\text{Im}E = \Gamma/2 = \pi \langle \Psi_{Eb} | H | \Psi_{Es} \rangle^2$$

with the total Hamiltonian $H$. The state functions $\Psi_{Eb}$ and $\Psi_{Es}$ are assumed to be normalized to 1 and by the $\delta(k-k')$ condition, accordingly. The matrix elements $\langle \Psi_{Es} | H | \Psi_{Es} \rangle$ entering the high-order PT corrections can be determined in the same way. They can be expressed through the set of one-dimensional integrals, described in details in Refs. [56-58].

In contrast to the hydrogen atom, the non-relativistic Schrödinger equation for an electron moving in the field of the atomic core in many-electron atom (in particular, an alkali element) and a uniform external electric field does not allow separation of variables in the parabolic coordinates $\xi, \eta, \varphi$ [2]. One of the ways this problem could be related to the use of effective potentials, chosen in such a way (for example, in the Miller-Green approximation [51]) to achieve the separation of variables in the Schrödinger equation. Here the model potential approach [59,60] or the quantum defect approximation [57] can be used. One may introduce the ion core charge $\,z_*$ for the multielectron atom. According to standard quantum defect theory, the relation between quantum defect value $\,\mu_i$, electron energy $E$ and principal quantum number $n$ is: $\mu_i = m - z_*(-2E)^{-1/2}$. The quantum defect in the parabolic coordinates $\delta(n, n, m)$ is connected to the quantum defect value of the free ($\,\varepsilon = 0$) atom by the following relation [57]:

$$\delta(n, n, m) = (1/n) \sum_{j=m}^{n-1} (2l+1)(C_{JM}^{jm})^2 \mu_i, \quad J = (n-1)/2, \quad M = (n_1 - n_2 + m)/2.$$  

Using the quantum defect approximation allows to modify the OPT method for the non-H atoms. In general form speech is about solving the problem associated with the use of a screened Coulomb approximation and further taking into account the non-Coulomb potential of the atomic residue in the calculation of mixing levels of an atom in an external field. The details of this procedure are presented in Ref. [57]. Further let us underline that the whole computational procedure at known resonance energy $E$ and separation parameter $\,\beta$, 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 $f_{k\beta}, \, g_{k\beta}, \, f_{\varepsilon}, \, g_{\varepsilon}$, as well as the equations for the integrals to compute (16) etc. 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”) [3,56-59].

3. Some results and conclusions

We have applied the developed computational approach to calculating the complex energy eigenvalues representing the shifted and broadened 2s state of lithium atom as a function of electric field strength. Sahoo and Ho [45] performed the calculation on the basis of a complex absorbing potential (CAP) method. Themelis and Nicolaides [42] adopted \textit{ab initio} theory to compute the complex energy of multielectron atomic states. Their approach is based on the state-specific construction of a non-Hermitian matrix according to the form of the decaying-state eigenfunction which emerges from the complex eigenvalue Schrodinger equation (CESE) theory. Meng et al [40] has elaborated the B-spline based coordinate rotation (B-CR) approach. In Table 1 we present our data on the eigenvalues EE (in atomic units: a.u.) representing the shifted and broadened 2s state of lithium atom as a function of electric field strength (in a.u.).
Table 1. Complex eigenvalues representing the shifted and broadened 2s state of lithium atom as a function of the field strength, calculated by different methods (see text).

| Li 2s | B-CR [40] | B-CR [40] | CAP [45] | CAP [45] | CESE [42] | Semiclassical [42] | This work | This work |
|-------|-----------|-----------|-----------|-----------|-----------|-------------------|-----------|-----------|
| $\epsilon$ (a.u.) | $E_\epsilon$ (a.u.) | $\Gamma/2$ (a.u.) | $E_\epsilon$ (a.u.) | $\Gamma/2$ (a.u.) | $\Gamma/2$ (a.u.) | $\Gamma/2$ (a.u.) | $E_\epsilon$ (a.u.) | $\Gamma/2$ (a.u.) |
| 0.0050 | -0.20009 | – | -0.20019 | 7.20[-9] | – | 4.65[-11] | -0.20012 | – |
| 0.0055 | -0.20052 | 3.80[-10]* | -0.20062 | 7.45[-9] | 5.91[-10] | 7.77[-10] | -0.20055 | 5.45[-10] |
| 0.0060 | -0.20100 | 3.74[-9]* | -0.20109 | 8.85[-9] | 5.46[-9] | 7.99[-9] | -0.20103 | 4.94[-9] |
| 0.0065 | -0.20151 | 2.49[-8]* | -0.20161 | 3.14[-8] | 3.52[-8] | 5.66[-8] | -0.20154 | 3.16[-8] |
| 0.0070 | -0.20207 | 1.24[-7]* | -0.20217 | 1.61[-7] | 1.69[-7] | 3.00[-7] | -0.20211 | 1.52[-7] |
| 0.0075 | -0.20268 | 4.87[-7] | -0.20277 | 4.83[-7] | 6.49[-7] | 1.26[-6] | -0.20272 | 5.08[-7] |
| 0.0080 | -0.20333 | 1.57[-6] | -0.20342 | 1.48[-6] | 2.06[-6] | 4.37[-6] | -0.20336 | 1.73[-6] |
| 0.0090 | -0.20477 | 1.05[-5] | -0.20486 | 1.05[-5] | 1.33[-5] | 3.41[-5] | -0.20480 | 1.21[-5] |
| 0.0100 | -0.20642 | 4.50[-5] | -0.20651 | 4.77[-5] | 5.50[-5] | 1.72[-4] | -0.20645 | 4.81[-5] |
| 0.0125 | -0.21147 | 4.76[-4] | -0.21155 | 4.68[-4] | 5.46[-4] | 2.95[-3] | -0.21149 | 4.96[-4] |
| 0.0150 | -0.21749 | 1.78[-3] | -0.21754 | 1.76[-3] | 1.97[-3] | 1.82[-2] | -0.21751 | 1.83[-3] |
| 0.0175 | -0.22393 | 4.03[-3] | -0.22397 | 4.06[-3] | 4.35[-3] | 6.35[-2] | -0.22394 | 4.24[-3] |

For comparison the analogous results, obtained on the basis of the CAP, CESE, B-CR methods [40,42,45] are presented. Analysis of the data shows that the positions (energies) of the Stark resonances in the present calculation are in a physically reasonable agreement with theoretical data obtained by other, in particular, CESE and B-CR methods. However, the results for the width of resonance differ more significantly from each other. For example, the CAP calculation for the width of the 2s state at strength $F < 0.0060$ a.u. gives systematically larger values than obtained by the CESE, B-CR and our methods. The resonance width values are higher than the corresponding B-CR data and correspondingly a little less than the values, obtained within the CESE method for all strengths of the electric field under consideration. Concerning the widths of resonances it should paid to attention on convergence aspect for the CAP and CESE method. As it has been underlined in [40], in the case of a weak electric field (naturally the widths of resonances became very small), the methods have difficulties in obtaining a stable value of a width. In order to obtain the well-converged results, it is necessary to use larger basis size. Naturally, in a limit of a weak electric field the well-known quasiclassical WKB approximation and standard PT [1,2] calculation will be more appropriate. One of the advantages of the B-CR method is possibility to apply in the case of increasing field strengths without a significant computational effort growth, however, the convergence of the width $\Gamma$ to obtain reliable complex eigenvalues should be carefully carried out. In the CAP method, there is no systematic way of choosing a scaling factor in an quite artificial complex potential, which is added to the original atomic Hamiltonian. One of the serious advantages of the modified OPT method is that an increasing a field strength does not lead to an increase of computational effort and there is no a convergence problem. The approach provides not only resonance state function definition but also the construction of the complex EE state function along with its complete orthogonal complementary of the scattering functions. In Refs. [63,64] the operator PT ideology has been used to consider a problem of resonances in the heavy ions collisions and AC Stark effect. The OPT approach can be used in calculating the Stark resonance parameters in a case of the strong electric fields and it is of a great interest for many modern atomic and molecular physics applications.

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