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SPECTROSCOPY OF MULTIELECTRON ATOM IN A DC ELECTRIC FIELD: MODIFIED OPERATOR PERTURBATION THEORY APPROACH TO STARK RESONANCES

It is presented a new modified method to calculation of the Stark resonances energies characteristics (energies and widths) for the multielectron atomic systems in a DC electric field. The method is based on the modified operator perturbation theory. The latter allows an accurate, consistent treatment of a strong field DC Stark effect and includes the physically reasonable distorted-waves approximation in the frame of the formally exact quantum-mechanical procedure. As illustration, some test data for the Stark resonances energies and widths in the lithium atom spectrum are presented and compared with results of calculations within the alternative consistent sophisticated methods.

1. Introduction

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) and by many applications on atoic, laser and plasmas physics [1-54].

An external electric field shifts and broadens the bound state atomic levels. The standard quantum-mechanical approach relates the complex eigenenergies (EE) 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. [1]) are introduced by Stebbings and Dunning, Kondratovich and Ostrovsky, Popov et al. Ivanov-Letokhov [5] have fulfilled the first estimations of the effectiviness 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 (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 ans Grecchi 1980, Maquet et al 1983, Kolosov 1987, Telnov 1989, Anokhin-Ivanov 1994), complex-coordinate method, quantum defect approximation etc (see review in Ref. [1]).

Hehenberger, McIntosh and E. Brändas [10] have applied the Weyl's theory to the Stark effect in the hydrogen atom.

Themelis and Nicolaides [42] adopted an *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 Schrodinger equation (CESE) theory. Sahoo and Ho [45] carried out the calculation the Stark resonances energies and widths in the lithium atom on the basis of the complex absorbing potential (CAP) formalism. Jianguo Rao et al and Hui-Yan Meng et al [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.[5,16] 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 of an atom in a strong DC electric field. **ë**

In this work we present a new modified version of the OPT method for the non-H atomic systems and test it by studying the Stark resonances parameters for some lithium atom states in a DC electric field. Besides, a relativistic generalization is presented too. 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 to Stark resonances for atoms in a DC electric field

As usually [16,47], 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^4/h^2) is:

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

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 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:

$$\psi(\zeta,\eta,\varphi)=f(\zeta)\, g(\eta)(\zeta\cdot\eta)^{|m|/2}\cdot \exp(im\varphi)/(2\pi)^{1/2} \quad (2)$$

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:

(5)

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 axis, and , at a given energy E are the solutions of the quadratic equation ( ):

$$t_2=\{[\ E^2_0 - 4\varepsilon(1-\beta)]^{1/2} - E_0\ \}/\varepsilon, \quad (6)$$

$$t_1=\{-[E^2_0 - 4\varepsilon(1-\beta)]^{1/2} - E_0\ \}/\varepsilon, \quad t_1< t_2 \quad (7)$$

To simplify the calculational procedure, the uniform electric field in (3) and (4) should be substituted by the function [16]:

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

with sufficiently large t (t=1.5t_2). The motivation of a choice of the $\varepsilon(t)$ and some physical features of electron motion along the h-axis are

presented in Refs. [1,2,16]. Here we only underline that the function $\varepsilon(t)$ practically coincides with the constant in the inner barrier motion region, i.e. < and disappears at > . It is important that the final results do not depend on the parameter *t*. It is carefully checked in the numerical calculation. 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 are possible. The latter are determined by the confinement condition for the motion along the *h*-axis. The same is true in our case, but only for $E \subset \left(-\frac{1}{2}\varepsilon, +\frac{1}{2}\varepsilon\right)$. 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 [2].

The total Hamiltonian $H(\varsigma, \nu, \varphi)$ does not possess the bound stationary states. According to OPT [16]), 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 G of the concrete quasistationary state in the lowest PT order one needs only two zeroth–order EF of H_0: bound state function $\Psi_{Б}(\varepsilon, \eta, \varphi)$ and scattering state function $\Psi_{К}(\varepsilon, \eta, \varphi)$ 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 with E $\subset \left(-\frac{1}{2}\varepsilon, +\infty\right)$. 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 [16]. The system (3) and (4) with the total Hamiltonian is solved under the conditions:

$$f(\mathrm{t}) \to 0 \text{ at } t \Rightarrow \infty, \qquad (9)$$

$$\partial x(\beta, E) / \partial E = 0 \text{ with}$$

$$x(\beta, E) = \lim_{t \Rightarrow \infty} [\, g^2(t) + \{g'(t) / \mathrm{k}\}^2 \,]\, t^{|m|+1}. \qquad (10)$$

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

$$\psi_{Eb}(\zeta, \eta, \varphi) = f_{Eb}(\zeta)\, g_{Eb}(\eta)(\zeta\eta)^{|m|/2} \\ exp\,(im\varphi)(2\pi)^{-1/2}, \qquad (11)$$

where $f_{Б}(t)$ is the solution of (3) (with the just determined E,) at $t \subset (0, \infty)$ and $g_{Б}(t)$ is the solution of (4) (with the same E,) at (inside barrier) and $g(t) = 0$ otherwise.

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

$$\psi_{E's}(\zeta, \eta, \varphi) = f_{E's}(\zeta)\, g_{E's}(\eta)\, (\zeta\eta)^{|m|/2} \\ \exp\,(\mathrm{i}m\varphi)(2\pi)^{-1/2} \qquad (12)$$

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. , must satisfy the equation (4) asymptotically. Following the OPT ideology [16], we choose the next form of , :

$$g_{E's}(t) = g_1(t) - z_2' g_2(t) \qquad (13)$$

with , 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 $\Rightarrow \infty$. The total equation system, determining the scattering function, reads

$$f'_{E's} + \frac{|m|+1}{t} f_{E's} + [1/2E' + (\beta_1' - \mathrm{N}/\mathrm{Z})/t - 1/4\ \varepsilon(\mathrm{t})t] \\ f_{E's} = 0, \\ g_1'' + \frac{|m|+1}{t} g_1' + [1/2E' + \beta_2'/t + 1/4\varepsilon(t)t] g_1 = 0, \\ g_2'' + \frac{|m|+1}{t} g_2' + [1/2E + \beta_2'/t + 1/4\varepsilon(\mathrm{t})\mathrm{t}] g_2 = 2g_{Eb}, \qquad (14)$$

(′ ′). At the given ′, the only quantum parameter ′ is determined by the natural boundary condition: $f_{E¢s}$Þ0 at t Þ ¥. Of course: ′ , $f_{E's} = f_{Б}$ at ′ ; only this case is needed in the particular problem we deal with here. The coefficient ′ ensures the orthogonality condition:

$$\langle \Psi_{Б} | \Psi_{E's} \rangle = 0 . \qquad (15)$$

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

$$\mathrm{Im}E = \mathrm{G}/2 = p|<Y_{Eb}|H|Y_{Es}>|^2 \qquad (16)$$

with the total Hamiltonian . The state functions $\Psi_{Б}$ and $\Psi_{Б}$ are assumed to be normalized to 1 and by the $\delta(k-k')$ condition, accordingly. The matrix elements $\langle \Psi_{Б} | H | \Psi_{E's} \rangle$ 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. [1,16].

In contrast to the hydrogen atom, the nonrelativistic 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 x, h, j [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; look review in ref [2]) that to achieve the separation of variables in the Schrödinger equation. Here the model potential approach [2] is used. One may introduce the ion core charge for the multielectron atom. According to standard quantum defect theory, the relation between quantum defect value , electron energy E and principal quantum number n is: $\mu_1 = \dot{o} - z^*(-2E)^{-1/2}$. The quantum defect in the parabolic coordinates $\delta(n_1 n_2 m)$ is connected to the quantum defect value of the free $(\varepsilon = 0)$ atom by the following relation [25,47]:

$$\delta(n_1 n_2 m) = (1/n)\sum_{l=m}^{n-1}(2l+1)(C^{JM}_{J,M-mlm})^2 \mu_l , \qquad (17)$$

Using the quantum defect approximation allows to modify the OPT method for the non-H atoms. All calculations are performed on the basis of the numeral code Superatom-ISAN (version 93). The details of the used method can be found in the references [1,2,16,25,47].

3. 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 *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 for 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]
ε (a.u.)	E_r (a.u.)	Γ/2 (a.u)	E_r (a.u.)	Γ/2 (a.u)
0.0050	−0.20009	–	−0.20019	7.20[−9]
0.0100	−0.20642	4.50[−5]	−0.20651	4.77[−5]
0.0125	−0.21147	4.76[−4]	−0.21155	4.68[−4]
0.0175	−0.22393	4.03[−3]	−0.22397	4.06[−3]
Li 2s	CESE [42]	WKB [42]	This work	This work
ε (a.u.)	Γ/2 (a.u)	Γ/2 (a.u)	E_r (a.u.)	Γ/2 (a.u)
0.0050	–	4.6[−11]	−0.20012	7.80[−9]
0.0100	5.50[−5]	1.72[−4]	−0.20645	4.81[−5]
0.0125	5.46[−4]	2.95[−3]	−0.21149	4.96[−4]
0.0175	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 Γ 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.

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SPECTROSCOPY OF MULTIELECTRON ATOM IN A DC ELECTRIC FIELD: MODIFIED OPERATOR PERTURBATION THEORY APPROACH TO STARK RESONANCES

Summary

It is presented a new modified method to calculation of the Stark resonances energies characteristics (energies and widths) for the multielectron atomic systems in a DC electric field. The method is based on the modified operator perturbation theory. The latter allows an accurate, consistent treatment of a strong field DC Stark effect and includes the physically reasonable distorted-waves approximation in the frame of the formally exact quantum-mechanical procedure. As illustration,

some test data for the Stark resonances energies and widths in the lithium atom spectrum are presented and compared with results of calculations within the alternative consistent sophisticated methods.

Keywords: multielectron atom in a dc electric field – modified operator perturbation theory – Stark resonances

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СПЕКТРОСКОПИЯ МНОГОЭЛЕКТРОННОГО АТОМА В DC ЭЛЕКТРИЧЕСКОМ ПОЛЕ: МОДИФИЦИРОВАННЫЙ МЕТОД ОПЕРАТОРНОЙ ТЕОРИИ ВОЗМУЩЕНИЙ ДЛЯ ОПИСАНИЯ ШТАРКОВСКИХ РЕЗОНАНСОВ

Резюме

Представлен новый модифицированный метод расчета характеристик энергий штарковских резонансов (энергии и ширины) для многоэлектронных атомных систем в электрическом поле. Метод основан на модифицированной операторной теории возмущений, которая обеспечивает последовательное, корректное описнаие эффекта Штарка в сильном поле для многоэлектронных атомов и базируется на использовании физически обоснованного приближения искаженных волн в рамках формально точной квантово-механической процедуры. В качестве иллюстрации представлены некоторые тестовые данные для энергий и ширин резонансов Штарка в спектре атомов лития, которые сравниваются с результатами расчетов в рамках альтернативных последовательных теоретических методов.

Ключевые слова: Многоэлектронный атом в электрическом поле – модифицированная операторная теория возмущений – штарковские резонансы

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СПЕКТРОСКОПІЯ БАГАТОЕЛЕКТРОННОГО АТОМА В DC ЕЛЕКТРИЧНОМУ ПОЛІ: МОДИФІКОВАНИЙ МЕТОД ОПЕРАТОРНОЇ ТЕОРІЇ ЗБУРЕНЬ ДЛЯ ОПИСУ ШТАРКІВСЬКИХ РЕЗОНАНСІВ

Резюме

Представлений новий модифікований метод розрахунку характеристик енергій штарківських резонансів (енергії і ширини) для багатоелектронних атомних систем в електричному полі. Метод заснований на модифікованій операторної теорії збурень, яка забезпечує послідовний, коректний опис ефекту Штарка в сильному полі для багатоелектронних атомів і базується на використанні фізично обґрунтованого наближення перекручених хвиль в рамках формально точної квантово-механічної процедури. В якості ілюстрації представлені деякі тестові дані для енергій і ширин резонансів Штарка в спектрі атомів літію, які порівнюються з результатами розрахунків в рамках альтернативних послідовних теоретичних методів.

Ключові слова: багатоелектронний атом у електричному полі – модифікована операторна теорія збурень – штарківські резонанси