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Calculations of relativistic Stark energies and widths in hydrogen-like ions using the complex-scaling method

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The relativistic calculations of energies and widths are performed for the lowest states of hydrogen and hydrogen-like neon. The calculations are carried out using the finite-basis technique combined with the complex-scaling method. The obtained results are compared with the available nonrelativistic and relativistic data.

Keywords: Stark effect, complex scaling.

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Introduction

Bound states of an atom or ion placed in a homogeneous electric field are shifted and turn into resonances having nonzero width and hence finite lifetime. Such phenomena is referred to as Stark effect and has been studied for a long time both experimentally [1–6] and theoretically [7–28]. However, most of the theoretical studies are devoted to nonrelativistic calculations. It shall be noted that relativistic effects may be of importance even in case of a hydrogen atom [23], but for heavy ions, only relativistic calculations can give accurate results. Moreover, precision experiments with heavy multicharged ions in very strong electric fields will become possible in the very near future. For example, such experimental research will be feasible within the Gamma Factory project [29]. It is expected that the Stark effect will be used to handle the heavy ion levels in a pre-defined way. Accurate theoretical positioning of these levels is essential for such research. Moreover, level widths are required to estimate the ion beam stability in strong magnetic fields.

Relativistic calculations of Stark resonance positions using the perturbation theory were carried out in [8]. In [28], a finite basis set was used to calculate the relativistic Stark shift in the hydrogen atom and hydrogen-like argon. It should be noted that the accuracy of methods based on the Hermitian Hamiltonian representation in the finite basis is limited because the resonance wave functions are not square integrable as opposed to the basis functions. In addition, such methods do not allow to calculate the resonance width (ionization probability per unit time). The relativistic Stark resonance width for hydrogen-like ions was calculated in [21,22] using quasi-classical approximation. Accuracy of such approximation, however, is also limited.

High-precision values for both resonance position and resonance width may be obtained by the complex-coordinate rotation method. This method involves rotation of a radial coordinate to a complex plane. After the rotation, the resonance wave functions become square integrable which enables to use standard methods based on the use of the finite basis set. In this case Hamiltonian loses Hermiticity and its intrinsic energies corresponding to resonances take complex values. Real part of such complex energy corresponds to the resonance position and imaginary part determines the resonance width. The relativistic complex-coordinate rotation method has been successfully used before to calculate auto-ionization states of multielectron ions [30–33] and supercritical resonance parameters in heavy quasi-molecules [34–37]. Description of the complex-coordinate rotation method and its variations may be found in [38,39].

To calculate the Stark energies and widths, the relativistic complex-coordinate rotation method was used in [23]. The calculations were carried out for lower states of the hydrogen atom and hydrogen-like neon ion. According to the obtained results, a conclusion was made regarding the significance of the relativistic effects even for hydrogen, in particular for relatively low electric field strengths. It was found that with a decrease in the electric field strength, the relativistic widths begin to exceed the nonrelativistic ones. This result differs qualitatively from the conclusion in [21,22] which is based on quasi-classical calculations and according to which relativistic widths are lower than nonrelativistic ones at low electric field strengths.

The purpose of the research was to settle the existing contradiction in the theoretical results and study the influence of the relativistic effects on the Stark resonance positions and widths. For this purpose, relativistic calculations for the hydrogen atom and hydrogen-like neon ion were carried out. The calculations were carried out in the finite basis set using the complex-coordinate rotation method. The obtained results were compared with the corresponding values from [23].

The Planck constant is assumed $\hbar = 1$ herein.

Theory and calculation methods

The relativistic spectrum of the hydrogen-like ion is calculated using the Dirac steady-state equation:

$$H\psi(\mathbf{r}) = E\psi(\mathbf{r}) \tag{1}$$

and in the presence of homogeneous electric field, Hamiltonian is as follows:

$$H = c(\boldsymbol{\alpha}\cdot\mathbf{p}) + V_{\text{nucl}}(r) - eFz + \beta m_e c^2. \tag{2}$$

Here, e is the electron charge ($e < 0$), c the speed of light, $(\boldsymbol{\alpha}, \beta)$ are Dirac matrices, $V_{\text{nucl}}(r)$ is the nucleus potential, the electric field with strength F is assumed to be directed along axis z. A uniformly charged sphere model is used herein for the nucleus potential:

$$V_{\text{nucl}}(r) = \begin{cases} \dfrac{eZ}{2R_{\text{nucl}}}\left(3 - \dfrac{r^2}{R_{\text{nucl}}^2}\right), & r < R_{\text{nucl}}, \\ \dfrac{eZ}{r}, & r > R_{\text{nucl}}, \end{cases} \tag{3}$$

where R_{nucl} is the nucleus radius.

The Dirac equation is used in the spherical coordinate system (r, θ, φ). Hamiltonian (2) is axially symmetrical about z axis, as a result the total angular momentum projection m on this axis is retained and the azimuth angle φ may be separated from the rest coordinates. Separation of variables may be carried out by substitution of the following function

$$\psi_m(r, \theta, \varphi) = \frac{1}{r}\begin{pmatrix} G_1(r,\theta)\exp\left[i\left(m - \frac{1}{2}\right)\varphi\right] \\ G_2(r,\theta)\exp\left[i\left(m + \frac{1}{2}\right)\varphi\right] \\ iF_1(r,\theta)\exp\left[i\left(m - \frac{1}{2}\right)\varphi\right] \\ iF_2(r,\theta)\exp\left[i\left(m + \frac{1}{2}\right)\varphi\right] \end{pmatrix} \tag{4}$$

in the Dirac equation (1). After such substitution, the Dirac equation can be reduced to the following form:

$$H_m\Phi(r,\theta) = E\Phi(r,\theta). \tag{5}$$

Here, the four-component wave function $\Phi(r, \theta)$ is as follows

$$\Phi(r,\theta) = \begin{pmatrix} G_1(r,\theta) \\ G_2(r,\theta) \\ F_1(r,\theta) \\ F_2(r,\theta) \end{pmatrix}, \tag{6}$$

and Hamiltonian H_m can be expressed as follows

$$H_m = \begin{pmatrix} m_e c^2 + V_{\text{nucl}} + eFz & c\,D_m \\ -c\,D_m & -m_e c^2 + V_{\text{nucl}} + eFz \end{pmatrix}, \tag{7}$$

$$\begin{aligned} D_m = {} & (\sigma_z\cos\theta + \sigma_x\sin\theta)\left(\frac{\partial}{\partial r} - \frac{1}{r}\right) \\ & + \frac{1}{r}(\sigma_x\cos\theta - \sigma_z\sin\theta)\frac{\partial}{\partial\theta} \\ & + \frac{1}{r\sin\theta}\left(im\sigma_y + \frac{1}{2}\sigma_x\right), \end{aligned} \tag{8}$$

where σ_x, σ_y and σ_z are Pauli matrices.

Due to the presence of a homogeneous electric field F, no bound states are present in the Hamiltonian spectrum (7). Instead, there are resonances which have a nonzero width Γ that determines the electron ionization probability. Since the resonance states do not belong to Hilbert space, they cannot be described by the square integrable basis functions. In order to overcome this problem, the complex-coordinate rotation method is used which is based on rotation of a radial coordinate to a complex plane. As a result of such rotation, the resonance wave functions become square integrable which enables to use standard methods of the finite basis set. We use herein a so called exterior complex scaling (ECS), when the radial coordinate is transformed as follows:

$$r \to \begin{cases} r, & r \le r_0, \\ r_0 + (r - r_0)e^{i\Theta}, & r > r_0, \end{cases} \tag{9}$$

where parameter r_0 is chosen so that with $r > r_0$ the potential in question is an analytic function. Thus, for potential (3), condition $r_0 \ge R_{\text{nucl}}$ shall be satisfied. In all calculations described herein, $r_0 = R_{\text{nucl}}$ was assumed.

After the transformation (9), Hamiltonian intrinsic energies (7) corresponding to resonances take complex values:

$$E_{\text{CS}} = E - i\Gamma/2. \tag{10}$$

Real part E of this quantity corresponds to the resonance position and imaginary part determines the resonance width Γ.

Solutions of the Dirac equation rotated to the complex plane are found using the finite basis set. The wave function $\Phi(r, \theta)$ is expanded in the basis:

$$\Phi(r,\theta) = \sum_{n=1}^{N} C_n W_n(r,\theta). \tag{11}$$

Basis functions $W_n(r, \theta)$ are constructed from B-splines according to the dual kinetic balance (DKB) method for axial symmetry systems [28]. The DKB technique prevents spurious states in the spectrum [40,41]. The basis construction method is described in detail in [42]. By substituting the expansion (11), the Dirac equation (5) is reduced to a finite-dimensional generalized eigenproblem which is solved using standard numerical procedures.

Results and discussion

Only states with the total angular momentum projection $m = 1/2$ were addressed herein. Complex energies E_{CS} were calculated by the method mentioned above. Resonance positions and widths are derived from E_{CS} using the equation (10).

Accurate solutions of the rotated Dirac equation do not depend on the complex rotation method Θ. However, the solutions obtained in the finite basis have such dependence.

Table 1. Position E and width Γ of the ground state of a hydrogen atom in a homogeneous electric field as function of field strength F

F, a.u.	Ref.	Relativistic		Nonrelativistic	
		E, a.u.	Γ, a.u.	E, a.u.	Γ, a.u.
0.01	a	$-0.50023220(1)$			
	b	-0.50023223		-0.5	0
0.02	a	$-0.50091583(1)$			
	b	-0.50091585		-0.5	0
0.03	a	$-0.50208081(1)$	$2.236(2) \cdot 10^{-8}$		
	b	-0.50208083		-0.50207427	
	c			-0.50207427	$2.23752 \cdot 10^{-8}$
0.04	a	$-0.50377803(1)$	$3.8913(9) \cdot 10^{-6}$		
	b	-0.50377804	$4.1 \cdot 10^{-6}$	-0.50377159	$3.9 \cdot 10^{-6}$
0.05	a	$-0.50611171(1)$	$7.7163(1) \cdot 10^{-5}$		
	b	-0.50611173	$7.74 \cdot 10^{-5}$	-0.50610543	$7.72 \cdot 10^{-6}$
0.06	a	$-0.50920954(1)$	$5.1496(1) \cdot 10^{-4}$		
	b	-0.50920955	$5.152 \cdot 10^{-4}$	-0.50920345	$5.151 \cdot 10^{-4}$
0.07	a	$-0.51308262(1)$	$1.8470(1) \cdot 10^{-3}$		
	b	-0.51308260	$1.8473 \cdot 10^{-3}$	-0.51307677	$1.8474 \cdot 10^{-3}$
0.08	a	$-0.51756625(1)$	$4.53896(3) \cdot 10^{-3}$		
	b	-0.51756619	$4.5391 \cdot 10^{-3}$	-0.51756062	$4.5397 \cdot 10^{-2}$
0.09	a	$-0.52241824(1)$	$8.78282(2) \cdot 10^{-3}$		
	b	-0.52241821	$8.7828 \cdot 10^{-3}$	-0.52241281	$8.7840 \cdot 10^{-3}$
0.1	a	$-0.52742345(1)$	$1.453646(3) \cdot 10^{-2}$		
	b	-0.527423540	$1.45362 \cdot 10^{-2}$	-0.52741818	$1.45381 \cdot 10^{-2}$

Note. a — this publication, b — publication [23], c — publication [18].

In order to improve convergence in the number of basis functions, it is a good practice to make calculations with an optimum complex rotation angle Θ_{opt} that corresponds to the minimum of derivative $|dE/d\Theta|$. It should be noted that Θ_{opt} takes different values for different states.

The calculations consisted of two stages. At the first stage, optimum angles Θ_{opt} were found using calculations in a small basis. At the second stage, the calculations were made using only optimum complex rotation angle. In this case, the calculations were carried out using bases of various sizes in order to define the final error. The error calculation procedure is described in detail in [32,33].

The results obtained for the ground state of a hydrogen atom are listed in Table 1. The appropriate relativistic and nonrelativistic values from [18,23] are also given for comparison. As can be seen from in the Table, the results obtained herein match well with the values in [23] at a high field strength F. However, at a relatively weak field, the calculated widths are repeatedly lower than the relativistic values from [23] and closer to nonrelativistic values. When $F < 0.03$ a.u., the accuracy of the used method is not enough in order to get the width values.

Table 2 shows the results for states $2s$, $2p_{1/2}$ and $2p_{3/2}$ of the hydrogen-like neon ion ($Z = 10$). For some F values, there are slight differences in the resonance positions between this publication and [23]. It should be noted that [23] used a point nucleus model, while the calculations described herein use the uniformly charged sphere model which enables to take into account the finite nuclear size. However, the influence of the finite nuclear size is negligible in this case and, though it is responsible for the difference in the resonance positions to some extent, it cannot account for the significant difference in the relativistic widths. It can be seen in the Table that the widths obtained herein are always lower than the nonrelativistic widths. Moreover, the relative difference between the relativistic and nonrelativistic results increases with a decrease in the field strength. In this case, with the decrease in the field strength, values from [23] begin to demonstrate the inverse trend at some moment and the relativistic width becomes higher than the nonrelativistic one. It should be noted that the relative reduction of the relativistic width with the decrease in the field strength matches with the conclusions in [21,22] which were based on the calculations with quasi-classical approximation.

Conclusion

Relativistic calculations of positions and widths of the lower states of a hydrogen atom and hydrogen-like neon ion in a homogeneous electric field have been carried out. The calculations have been made using the finite basis set method with complex rotation technique. Some of the obtained results do not match the corresponding values from [23]. The cause of the difference is not clear. All obtained relativistic widths are lower than the corresponding nonrelativistic ones and the relative difference increases with the decrease in the electric field strength. Qualitatively, this

Table 2. positions E and widths Γ of lower excited states of a hydrogen-like ion ($Z = 10$) in a homogeneous electric field as function of field strength F

F, a.u.	Ref.	Relativistic		Nonrelativistic	
		E, a.u.	Γ, a.u.	E, a.u.	Γ, a.u.
		$2s_{1/2}$			
2	a	$-12.546703(1)$			
	b	-12.54670		-12.53157	0
4	a	$-12.646250(1)$	$7.790(1) \cdot 10^{-5}$		
	b	-12.64625	$8 \cdot 10^{-5}$	-12.63169	$8 \cdot 10^{-5}$
6	a	$-12.840441(1)$	$2.1280(1) \cdot 10^{-2}$		
	b	-12.84044	$2.126 \cdot 10^{-2}$	-12.82715	$2.178 \cdot 10^{-2}$
8	a	$-13.138005(1)$	$2.04167(2) \cdot 10^{-1}$		
	b	-13.13801	$2.0423 \cdot 10^{-1}$	-13.12615	$2.0731 \cdot 10^{-1}$
10	a	$-13.463513(1)$	$6.21217(1) \cdot 10^{-1}$		
	b	-13.46349	$6.214 \cdot 10^{-1}$	-13.45247	$6.2792 \cdot 10^{-1}$
		$2p_{1/2}$			
2	a	$-13.149636(1)$			
	b	-13.14961	$2 \cdot 10^{-5}$	-13.13533	$1 \cdot 10^{-5}$
4	a	$-13.867642(1)$	$4.2833(4) \cdot 10^{-4}$		
	b	-13.86772	$4.4 \cdot 10^{-4}$	-13.85488	$4.5 \cdot 10^{-4}$
6	a	$-14.719703(1)$	$6.5523(1) \cdot 10^{-2}$		
	b	-14.71966	$6.554 \cdot 10^{-2}$	-14.70918	$6.676 \cdot 10^{-2}$
8	a	$-15.674145(1)$	$4.27531(1) \cdot 10^{-1}$		
	b	-15.67420	$4.2773 \cdot 10^{-1}$	-15.66554	$4.3223 \cdot 10^{-1}$
10	a	$-16.616918(1)$	$1.08062(1)$		
	b	-16.61683	1.08039	-16.60929	1.08833
		$2p_{3/2}$			
2	a	$-11.948679(1)$			
	b	-11.94869	$2 \cdot 10^{-5}$		$1 \cdot 10^{-5}$
4	a	$-11.446913(1)$	$1.426(2) \cdot 10^{-5}$		
	b	-11.44692	$3 \cdot 10^{-5}$	-11.43054	$2 \cdot 10^{-5}$
6	a	$-11.019910(1)$	$5.9228(6) \cdot 10^{-3}$		
	b	-11.01991	$5.93 \cdot 10^{-3}$	-11.00366	$6.09 \cdot 10^{-3}$
8	a	$-10.683798(1)$	$8.4307(3) \cdot 10^{-2}$		
	b	-10.68390	$8.444 \cdot 10^{-2}$	-10.66829	$8.619 \cdot 10^{-2}$
10	a	$-10.404716(1)$	$3.23139(1) \cdot 10^{-1}$		
	b	-10.40443	3.2374	-10.38915	3.2853

Note. a — this publication, b — publication [23].

result matches the conclusions in [21,22] obtained within the quasi-classical approximation.

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Conflict of interest

The authors declare that they have no conflict of interest.

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