Eur. Phys. J. D **38**, 471–479 (2006)
DOI: 10.1140/epjd/e2006-00061-y

**THE EUROPEAN
PHYSICAL JOURNAL D**

Helium atom in presence of DC and AC electric fields

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Received 29 November 2005

Abstract. We investigate the effect of a static electric field on photoionization of the He atom in the ground 1S and low-lying 2S and 2P excited states. The field-affected ionization potential and photoionization cross-section are determined from the complex eigenvalues of the time-dependent Schrödinger equation solved by the complex rotation method in the Floquet ansatz. Accuracy of the method is enhanced by the use of the Hylleraas basis set. For the ground state of helium, we find that the total photoionization cross-section remains constant or decreases as a function of the DC field strength until this field reaches a certain critical value. For the low-lying excited states, effect of the static field is similar to the ordinary DC Stark effect.

PACS. 32.80.-t Photon interactions with atoms – 32.80.Fb Photoionization of atoms and ions – 42.50.Hz Strong-field excitation of optical transitions in quantum systems; multiphoton processes; dynamic Stark shift

1 Introduction

The effect of an external DC electric field on the process of interaction of a two-electron atomic system and AC electromagnetic field has become a subject of intense experimental and theoretical studies. For the hydrogen negative ion, for example, there is a wealth of both experimental [1,2] and theoretical [3–5] results concerning influence of the external DC electric field on the process of photodetachment.

Effect of a DC field on the photoionization from the ground state of helium was studied in [6–8]. These authors were interested in the photoionization cross-sections in the region of $2lnl'$ resonances. Due to the Stark mixing of the levels in the final state, application of the external DC field opens new photoionization channels. For example, in the absence of the external DC field the states of $^1\mathrm{D}^e$ symmetry cannot be reached via the process of one-photon ionization from the ground state. The external DC field mixes the states of the $^1\mathrm{D}^e$ and $^1\mathrm{P}^o$ symmetries and makes this process possible. It was found [6] that this effect leads to the redistribution of the photoionization rates between various final channels. Thus, for example, the photoionization cross-section for the $^1\mathrm{P}^o$ channel may decrease with the DC field, while, that for the $^1\mathrm{D}^e$ may increase. Experimentally, the effect of a static electric field on the resonant photoionization of He was recently studied [9]. This study lead to a discovery of a propensity rule for selective double photoexcitation of helium in DC fields [10].

In the cited theoretical works on the resonant photoionization of He, the AC field was treated perturbatively. A convenient framework for such a treatment is provided by the complex rotation method (CRM) [11]. Knowledge of the eigenvalues of the complex-rotated Hamiltonian allows one to construct a representation [12] for the projection operator on an interval of the continuous spectrum of the Hamiltonian of the system. This representation can then be used for efficient perturbative computation of the cross-sections.

In the view of the current interest in behavior of atomic systems in strong fields (see, e.g. [13]), non-perturbative techniques, suitable for describing response of atomic systems to strong external fields are becoming increasingly important.

Several approaches providing such a description for systems with more than one electron have been proposed in the literature. An approach based on the combination of R-matrix and Floquet techniques [14,15] allows to describe non-perturbatively behavior of multielectron atomic systems such as He [16], hydrogen negative ion [17]) or H_2 molecule [18] in the presence of strong AC fields.

Direct solution of the time-dependent Schrödinger equation (TDSE) for systems with more than electron in external laser field is also possible. Such procedure has been used to study effects of strong AC field on He [19] and molecular hydrogen [20]. An efficient method of solving the TDSE for two-electron systems has been presented in [21], allowing to consider processes of ionization and excitation by short laser pulses in helium and negative hydrogen ion. The multiconfiguration time-dependent Hartree-Fock approach, allowing to describe behavior of a

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few-electron system in the presence of the strong laser field was proposed recently [22]. The above methods provide, in principle, a comprehensive non-perturbative description of the behavior of the systems with at least two electrons in the presence of strong external AC fields.

Providing such a description for a multielectron system in the case of the external DC field requires a different set of ideas. One can try, for example, to combine the existing electronic structure theories (based e.g., on the single- or multi-configuration Hartree-Fock methods) with the methods suitable for the description of the decaying states [23,24]. This can be done, for example, in the spirit of the Feshbach projection operators formalism by introducing complementary Q and P spaces [25]. Alternatively, to determine total ionization rates and level shifts in multielectron systems in the presence of external DC field, one may use the complex rotation method. Justification of this method for the case of an atom in the presence of external DC field has been laid out in the pioneering works [26–28]. Once the validity of the CRM in this problem has been established, it became possible to use highly accurate matrix methods from the theory of the bound state calculations. Positions and widths of the Stark resonances in various systems (such as He, H^-, Ps^-) could thus be computed with accuracy comparable to the accuracy of the bound state calculations [29,30]. Further development these ideas received in the work [31] where the so-called exterior complex rotation method has been applied for the theoretical study of the ionization rates and Stark shifts of molecular hydrogen in external DC or low-frequency laser fields.

In the present paper we shall try to describe a two-electron system non-perturbatively in the presence of both AC and DC electric fields. As a theoretical tool, we also employ the CRM, albeit in a slightly different guise. We shall use the so-called Floquet ansatz to represent the wave function of the atom in the external monochromatic AC field. The resulting set of equations is solved with the use of the CRM by means of ordinary variational techniques. In this approach, both AC and DC fields are considered non-perturbatively.

A completely rigorous mathematical proof of the validity of the CRM in the present context is still lacking [32]. There is, however, a strong evidence supported by numerous successful applications to atomic systems like hydrogen [33–36], that the CRM in its usual form applies to the situations in which the AC electromagnetic field is present.

The net gain in applying the combination of the CRM and Floquet methods to the two-electron systems in external fields is the possibility to treat both the AC and DC fields non-perturbatively. This is an important advantage, especially in the view of the current interest in behavior of atomic systems in strong fields (see, e.g. [13]). To achieve this gain, however, one must overcome rather severe computational problems related to the size of the target state basis size. The obvious requirement to the basis set is an accurate description of the field-free atomic states and the ordinary DC Stark effect. Once this goal is achieved, the dimension of the matrices thus obtained is to be further increased to describe accurately the influence of the AC field (see more details below). The overall dimension of the problem may, therefore, make the whole approach impracticable. A solution of this problem is to choose the basis so that the DC Stark effect for each Floquet block is described as economically as possible, with the use of the minimal number of the basis functions. The Hylleraas basis set, well-known for its efficiency in representing field-free atomic states [37], is a natural choice here. We might mention also the work of [21] where this property of the Hylleraas basis to economize the dimension of the basis set has been used for the solution of the time-dependent Schrödinger equation for a two-electron system placed in external AC field.

An analogous approach to strong AC fields has been developed in [38] where the so-called perimetric coordinates have been used. The authors applied this approach to the negative hydrogen ion in a very strong AC field. In particular, they were able to estimate the onset of the AC stabilization for this system. Basis functions expressed in the perimetric coordinates (supplemented with the three Euler angles) constitute the basis which, from the formal point of view, is equivalent to the Hylleraas basis employed in the present paper. There is, however, one important difference. As it was noted [38], the approach based on the perimetric coordinates and Euler angles leads to considerable problems of technical character, especially if one attempts to construct a state with the large total angular momentum. For the strong external fields which mix various symmetries, an account of the states of large momenta can become quite important. The Hylleraas basis set, employing spherical coordinates for both electrons, is much easier to implement, in particular for the states with large angular momenta.

In our recent paper [39] we applied a combination of these techniques (CRM + Floquet + Hylleraas basis set) to describe helium atom placed in an external AC electric field. We have shown that the aforementioned combination of methods allows to achieve an unprecedented accuracy (on the level of a fraction of a percent) in determining the total photoionization cross-sections for the helium atom. In the present work we show how this approach can be applied for the considerably more complicated problem of helium atom in presence of both AC and DC electric fields. We shall be interested in photoionization of He outside the resonant region where a sufficiently strong external DC field can change the ionization potential and the photoionization cross-section. We shall report below results of an accurate non-perturbative calculation of the ionization potentials and the photoionization cross-sections of the He atom in the ground 1S state and lower-lying 2S and 2P singlet and triplet excited states. These parameters are extracted from the positions and widths of the corresponding decaying (resonant) states of the He atom in the presence of external DC and AC fields.

The paper is structured as follows. In Section 2 we present the formalism, introduce the Hylleraas basis set and outline our computational strategy. In Section 3 we compile our numerical results for the singlet and triplet states. We conclude by speculating on the possible use of the present technique for other related problems.

2 General theory

The non-relativistic Hamiltonian of the helium atom in the presence of the external monochromatic linearly-polarized AC electromagnetic field and the external DC electric field can be written as:

$$\hat{H} = \frac{\mathbf{p}_1^2}{2} + \frac{\mathbf{p}_2^2}{2} - \frac{2}{r_1} - \frac{2}{r_2} + \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} + \mathbf{D} \cdot (\mathbf{F}_{\mathrm{AC}} \cos \omega t + \mathbf{F}_{\mathrm{DC}}), \quad (1)$$

where $\mathbf{D} = \mathbf{r}_1 + \mathbf{r}_2$. In the present work we adopt the length gauge to describe interaction of the atom and the field. We also rely on the dipole approximation so that the quantity $\mathbf{F}_{\mathrm{AC}}$ is coordinate independent. Unless stated otherwise, the atomic units are used throughout the paper.

The theoretical method employed below is based on the work [33]. The time-dependent Schrödinger equation (TDSE) allows the following set of solutions in the so-called Floquet-Fourier ansatz [14,33,40,41].

$$\Psi(t) = e^{-iEt} \sum_n u_n e^{-inwt}. \quad (2)$$

Substituting this expression into the TDSE one obtains a chain of coupled equations for the coefficient functions u_n:

$$(E - \hat{T} - \hat{U} - \mathbf{D} \cdot \mathbf{F}_{\mathrm{DC}} + n\omega) u_n = \frac{\mathbf{F}_{\mathrm{AC}} \cdot \mathbf{D}}{2} (u_{n-1} + u_{n+1}), \quad (3)$$

where $n = 0, \pm 1 \ldots$, E, $\hat{T}$ and $\hat{U}$ stand, respectively, for the quasi-energy and the operators of kinetic and potential energy. To solve this set of equations we employ the complex rotation method (CRM) [11,32,42–45]. Formally, the CRM can be described as a complex transformation of radial variables $r_i \to r_i e^{i\theta}$, where θ is the so-called rotation angle, parameter defining the transformation.

Under this transformation, the chain of equations (3) is converted into

$$(E - \hat{T} e^{-2i\theta} - \hat{U} e^{-i\theta} - \mathbf{D} \cdot \mathbf{F}_{\mathrm{DC}} e^{i\theta} + n\omega) u_n = \frac{\mathbf{F}_{\mathrm{AC}} \cdot \mathbf{D}}{2} e^{i\theta} (u_{n-1} + u_{n+1}). \quad (4)$$

According to the general theory of CRM [11,42–44], the eigenvalue problem (4) can be solved by means of variational techniques if the rotation angle θ is properly chosen. The (complex) eigenvalues of this problem:

$$E = E_r - i \frac{\Gamma}{2} \quad (5)$$

provide information about the energy (E_r) and the width (or decay rate Γ) of the atomic state in the field.

In the case of very weak DC fields, when the decay due to the interaction with the AC field plays predominant role, the latter quantity can be related to the total photoionization cross-section (in a.u.) by means of a well-known relation:

$$\sigma = \lim_{F_{\mathrm{AC}} \to 0} \frac{8\pi\alpha\Gamma\omega}{F_{\mathrm{AC}}^2}. \quad (6)$$

As the limiting procedure in the last equation suggests, this equation is valid only if it is legitimate to consider the AC field perturbatively.

Below we shall consider the case when DC and AC electric field vectors are parallel, this direction we choose as the z-axis. We shall restrict our attention only to the manifold of states with $M = 0$, where M is a projection of the total orbital momentum on the quantization z-axis (in the present set-up M is a conserved quantity).

To solve the eigenvalue problem (4) variationally we introduce a basis set of square integrable functions $|n,k\rangle$ where the index n refers to the number of the Floquet block and the index k denotes a particular L^2 function in the subspace of the nth block so that $u_n = \sum_k c_{nk} |n,k\rangle$. With these notations, the set of equations (4) can be rewritten in a matrix form as:

$$\left((E + n\omega) R^{nk}_{n_1 k_1} - T^{nk}_{n_1 k_1} e^{-2i\theta} - U^{nk}_{n_1 k_1} e^{-i\theta}\right) c_{nk} = F_{\mathrm{DC}} D^{n_2 k}_{n_1 k_1} e^{i\theta} c_{nk} + \sum_{n2 = n \pm 1} F_{\mathrm{AC}} D^{n_2 k}_{n_1 k_1} \frac{e^{i\theta}}{2} c_{n_2 k}, \quad (7)$$

where it is understood that summation is carried over the repeated k-index. Here F_{AC} and F_{DC} are field strengths of the AC and DC electric fields, respectively, D is the matrix of the operator $D_z = z_1 + z_2$, and R, T and U stand for the overlap, kinetic energy and potential energy matrices, respectively.

In practical calculations we must, of course, truncate system (7), considering only a finite number of the Floquet blocks. In the present work, we consider only intensities of AC electromagnetic field not exceeding 0.1 a.u. For such AC field intensities the contribution of the Floquet blocks with $|n| > 1$ in equation (7) can be neglected. As usual in the variation calculations, this statement can be verified by performing extended calculation including, e.g., Floquet blocks with $n = \pm 2$. Such verification has been performed confirming the above statement. We shall give more details of this calculation below. For the moment we shall assume that in the region of the AC field strengths reported here it is legitimate to retain only the Floquet blocks with $|n| \leq 1$ in the set of equations (7).

Our next step is to choose the basis set $|n,k\rangle$ in (7). We employ the Hylleraas basis set consisting of the functions:

$$g_{n_1,n_2,N}(\mathbf{r}_1, \mathbf{r}_2) = r_1^{n_1}\ r_2^{n_2}\ |\mathbf{r}_1 - \mathbf{r}_2|^N \times e^{-ar_1 - br_2} |l_1(1) l_2(2) L\rangle, \quad (8)$$

where a, b are some constants (to be specified below), n_1, n_2, N are integers and the angular part

$$|l_1(1) l_2(2) L\rangle = \sum_{m_1 m_2} C^{LM}_{l_1 m_1 l_2 m_2} Y_{l_1 m_1}(\mathbf{n}_1) Y_{l_2 m_2}(\mathbf{n}_2), \quad (9)$$

represents two spherical functions (of orders l_1, l_2) coupled to represent a state with a given total angular momentum L. Of course, basis functions (8) must be properly symmetrized with respect to exchange of the electron coordinates. When choosing parameters in (8), we were guided by the following rule [29,37]. All the basis functions with the parameters satisfying the inequality (the so-called Pekeris shell)

$$n_1 + n_2 + N < N_{\max} \tag{10}$$

were included in the calculation. The parameter $N_{\max}$ determines the overall size of the basis. There is another well established rule for choosing angular momenta l_1, l_2 in (8). For states with the natural parity, l_1, l_2 are best chosen so that $l_1 + l_2 = L$. Both these criteria help to avoid the numerical problems due to near-degeneracy of the basis set when its dimension becomes large. Some details of the calculations of the Hamiltonian matrix with the functions (8) are given in the Appendix.

3 Numerical results

To describe accurately the helium atom in the presence of the DC electric field we use a sufficient number of basis functions of S, P, D, F, G and H symmetries to represent each Floquet block in system (7).

3.1 Singlet states

For the singlet states, the basis set satisfying the criteria mentioned above can be constructed as follows. Each of the parameters a, b in equation (8) was allowed to assume two values: 1 and 0.5. This is the so-called split exponential basis needed to describe accurately singly excited states $1s2l$ where there are two different radial scales. For each of the Floquet blocks in set (7) we retain all the basis functions of ${}^1\mathrm{S}^e$, ${}^1\mathrm{P}^o$, ${}^1\mathrm{D}^e$, ${}^1\mathrm{F}^o$, ${}^1\mathrm{G}^e$,${}^1\mathrm{H}^o$ symmetries for which the parameter $N_{\max}$ in (10) is equal to 9. Such a choice gives us for each Floquet block a total of 260, 336, 90, 70, 53 and 30 basis functions of ${}^1\mathrm{S}^e$, ${}^1\mathrm{P}^o$, ${}^1\mathrm{D}^e$, ${}^1\mathrm{F}^o$, ${}^1\mathrm{G}^e$ and ${}^1\mathrm{H}^o$ symmetries respectively. Since we consider only Floquet blocks with $n = 0, \pm 1$, the overall dimension of the eigenvalue problem (7) is 2517. All calculations reported below have been performed using quadruple precision arithmetic.

An estimate of the accuracy of the present calculation can be inferred from the field-free case when both the DC and AC fields are switched off. Such a calculation gives the following energies of the states of interest: -2.90372443 a.u. (the ground state), -2.14597414 a.u. (the $1s2s$ ${}^1\mathrm{S}^e$ state) and -2.12384295 a.u. (the $1s2p$ ${}^1\mathrm{P}^o$ state). Comparison with the well-known values from the literature [37,46] shows that we may claim an accuracy of the order of 10^{-7} a.u. for the ground and $1s2p$ ${}^1\mathrm{P}^o$ excited states, and 10^{-8} a.u. for the $1s2s$ ${}^1\mathrm{S}^e$ state. We can adopt the larger of these numbers as a conservative estimate of the accuracy our basis gives in the field-free case. Such an accuracy may not seem to be very impressive by the usual standards of the Hylleraas basis calculations but, as we mentioned above, we have to find a compromise between the accuracy and computational time since inclusion of several Floquet blocks increases the dimension of the eigenvalue problem (7). The quoted estimate of the accuracy will be found sufficient for the accurate calculation of the combined effects of DC and AC fields on these states.

Before proceeding to calculations with both the DC and AC fields included (that is, to the calculation including several Floquet blocks in (7)), we have yet to make sure that our basis describes accurately the ordinary DC Stark. To verify this, we put $F_{\mathrm{AC}} = 0$ in (7), restricted the system of equations to only one Floquet block (with $n = 0$), and diagonalized the resulting eigenvalue problem. The composition of the only Floquet block with $n = 0$ was the same as we described above. The results which this procedure gave for the positions and widths of the ground state and the excited $1s2s$ ${}^1\mathrm{S}^e$, $1s2p$ ${}^1\mathrm{P}^o$ states agree very well with the known literature values. For example, for the DC field strength $F_{\mathrm{DC}} = 0.05$ a.u. we obtained the ground state energy of -2.90546493 a.u. Comparing this value with the quoted above field-free result obtained in the same basis, we find a level shift of 0.00174 a.u. This result is to be compared with the value of 0.00175 a.u. obtained in the work [25]. For the DC field strength $F_{\mathrm{DC}} = 0.15$ a.u. we obtained the width of the ground state of 0.000417 a.u. which is to be compared to 0.000425 a.u. reported in the paper [24]. Thus, even for the DC field strengths as large as 0.15 a.u., our basis provides quite an adequate description of the DC Stark effect.

Having assured validity of the description which our basis provides for the field-free He atom and the DC Stark effect, we may proceed to a complete calculation including several Floquet blocks in (7). As we mentioned above, we included in the calculation the Floquet blocks with $n = 0, \pm 1$. To make sure that for the AC field strength considered (of the order of 0.1 a.u.) this choice provides an adequate approximation, we ran a calculation with $F_{\mathrm{DC}} = 0$, $F_{\mathrm{AC}} = 0.1$ a.u., retaining in equations (7) Floquet blocks with $n = 0, \pm 1, \pm 2$. The composition of the Floquet blocks was as described above with the difference, that for the case of $F_{\mathrm{DC}} = 0$ we may leave in the Floquet blocks with $n = 0, n \pm 2$ only even basis functions, and in the blocks $n = \pm 1$ only odd basis functions. Such calculation gave for the position and width of the ground state resonance -2.90338569 a.u. and 0.00014714 respectively, which agrees quite well with the data from the Table 1 obtained with the use of the Floquet blocks with $n = 0, \pm 1$.

All results reported below refer to the frequency of the AC electromagnetic field $\omega = 111$ eV. Our numerical results are listed in the Tables 1 (ground state) and 2 (excited states). To test the accuracy of these results, we performed a separate calculation retaining the Floquet blocks with $n = 0, n \pm 1, n \pm 2$ in system (7). The composition of each Floquet block in this calculation was as described above. Such calculation, performed for

Table 1. Energy and width (in a.u.) of the $1s^2\ ^1$S state of the helium atom in the presence of DC and AC electric fields (field strengths in a.u., $\omega = 111$ eV).

	$1s^2\ ^1$S	
$F_{\rm DC}$	E	Γ
	$F_{\rm AC} = 0.1$	
0	−2.9033858	1.4708-4
0.05	−2.9051265	1.4683-4
0.1	−2.9105049	1.4675-4
0.15	−2.9202165	5.6224-4
	$F_{\rm AC} = 0.13$	
0	−2.9031524	2.4849-4
0.05	−2.9048932	2.4803-4
0.1	−2.9102718	2.4746-4
0.15	−2.9199840	6.5271-4

Table 2. Energy and width (in a.u.) of the $1s2s\ ^1$S and $1s2p\ ^1$P sates of the helium atom in the presence of DC and AC electric fields (field strengths in a.u., $\omega = 111$ eV).

	$1s2s\ ^1$S		$1s2p\ ^1$P	
$F_{\rm DC}$	E	Γ	E	Γ
		$F_{\rm AC} = 0.05$		
0	−2.1458914	2.68-5	−2.1237419	2.06-4
0.0005	−2.1459910	2.78-5	−2.1236884	2.02-4
0.001	−2.1462856	3.15-5	−2.1234445	2.69-4
0.002	−2.1474064	5.81-5	−2.1225276	5.22-4
0.003	−2.1491111	1.316-4	−2.1211653	9.11-4
0.004	−2.1512526	2.710-4	−2.1195121	1.412-3
0.005	−2.1537179	4.851-4	−2.1177007	2.018-3
0.01	−2.1691494	2.8079-3	−2.1074370	6.7483-3
		$F_{\rm AC} = 0.1$		
0	−2.1456444	1.073-4	−2.1235583	7.028-4
0.0005	−2.1457441	1.106-4	−2.1234755	7.229-4
0.001	−2.1460361	1.210-4	−2.1231002	8.639-4
0.002	−2.1471592	1.710-4	−2.1223129	1.0124-3
0.003	−2.1488631	2.738-4	−2.1209489	1.3719-3
0.005	−2.1534658	6.837-4	−2.1174776	2.4209-3

$F_{\rm AC} = 0.1$ a.u. and $F_{\rm DC} = 0.005$ a.u. gave −2.1534632 a.u. and 0.0006848 a.u. (position and width of the $1s2s\ ^1$S state) and −2.1174750 a.u. and 0.0024231 a.u. (position and width of the $1s2p\ ^1$P state). This is to be compared with the results presented in the Table 2. It can be seen that the difference of these results does not exceed 5×10^{-6} a.u. For the ground state, variation of the results with respect to the number of the Floquet blocks was also found to be within these limits. Combining this estimate and the estimates presented above for the field-free case and ordinary DC Stark effect, we adopt the latter figure as an estimate for the accuracy of the data reported in the Tables 1, 2 and 3.

Figure 1 gives a graphical representation of the ground state energy and width as functions of the DC field strength for two different values of the AC field strength.

Most noticeable feature of this figure is that the width does not increase (or even decrease) as a function of the applied DC electric field until the field strength reaches some critical value (approximately 0.1 a.u.). The corresponding low DC-field value of the total photo-ionization cross-section, computed with the use of (6), coincides within a fraction of a percent with the experimental value [47].

Table 3. Energy and width (in a.u.) of the $1s2s\ ^3$S and $1s2p\ ^3$P states of the helium atom in the presence of DC and AC electric fields (field strengths in a.u., $\omega = 111$ eV).

	$1s2s\ ^3$S		$1s2p\ ^3$P	
$F_{\rm DC}$	E	Γ	E	Γ
		$F_{\rm AC} = 0.05$		
0	−2.1751464	2.71-5	−2.1330972	1.37-4
0.001	−2.1753039	2.79-5	−2.1330044	2.08-4
0.002	−2.1757721	3.26-5	−2.1327312	4.20-4
0.003	−2.1765385	4.82-5	−2.1322930	7.63-4
0.005	−2.1788889	1.514-4	−2.1310398	1.796-3
		$F_{\rm AC} = 0.1$		
0	−2.1748985	1.083-4	−2.1328972	5.379-4
0.001	−2.1750562	1.106-4	−2.1328036	6.084-4
0.002	−2.1755248	1.199-4	−2.1325282	8.172-4
0.003	−2.1762920	1.427-4	−2.1320865	1.157-3
0.005	−2.1786438	2.662-4	−2.1308210	2.179-3

The accuracy of the present calculation does not allow us to assert that the width indeed appreciably declines with DC electric field. It does allow us, however, to conclude that it remains virtually constant for the DC electric field strength below 0.1 a.u., starting to grow rapidly for larger field strengths. Such a behavior is reminiscent of the widths of doubly-excited resonance states of two-electron systems in the presence of the DC external field. It was found, for example, for the doubly excited resonance states in helium [48], negative hydrogen ion [30], positronium negative ion [49] or molecular hydrogen [31]. For these systems, such a behavior was explained as a result of a competition of two possible routes of decay (the autoionizing one and the one due to the presence of the DC field). In all these systems which are highly correlated atomic species, the interference of the two decay processes may lead to observed decrease of the width as a function of the DC field strength. It is only for larger field strengths that the DC field effect becomes dominant and we find a typical pattern of a monotonous growth of the width with field (found e.g., for hydrogen atom). It is quite possible that analogous situation occurs in the present case where the role of autoionization process is played by the ionization due to the presence of the AC field. To make this discussion more precise we should recall that for not very large field strengths there are two distinct processes which can lead to ionization of an atom by an external electric field. These processes are perturbative multiphoton ionization and tunneling. The third process, the so-called above barrier ionization, occurs for the field strengths far larger than those considered in the paper. Which process plays the major role is determined by the Keldysh parameter γ [50] which is proportional to

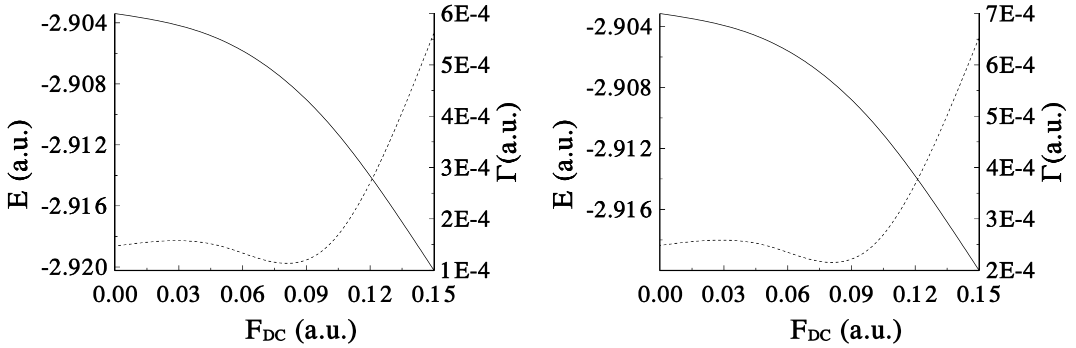

Fig. 1. Energy (solid line) and width (dashed line) (in a.u.) of the $1s^2\ ^1$S state of the helium atom as functions of the DC field strength. The AC field is applied with the frequency $\omega = 111$ eV and the field strength $F_{\rm AC} = 0.1$ a.u. (left) and 0.13 a.u. (right).

the frequency of the laser field. The case $\gamma \gg 1$ corresponds to the multiphoton ionization regime whereas in the opposite case $\gamma \ll 1$ the tunneling regime dominates. In the present case, both these mechanisms are equally important. It is easy to see that for the parameters of the AC field considered in the paper we have $\gamma \gg 1$, hence ionization due to AC field proceeds mostly by the multiphoton ionization process. The DC field ionization, on the contrary, proceeds by tunneling. The statement made above may therefore be reformulated as the following hypothesis. In some regions of the parameters characterizing the problem, the interference of these two processes may actually lead to the decrease of the total ionization width. To cast this hypothesis into somewhat more quantitative terms, we could use the so-called Kramers-Henneberger representation of the equations governing interaction of atom with the AC field [51–53]. We recall that this representation is equivalent to the use of the coordinate system oscillating with the frequency ω of the AC field: $\mathbf{r} \to \mathbf{r} + \alpha(t)$, where $\alpha = \mathbf{F}_{\rm AC}\cos\omega t/\omega^2$. Under this transformation the Hamiltonian operator (1) assumes the form:

$$\hat{H}_{\rm KH} = \hat{T} - \frac{2}{|\mathbf{r}_1 - \alpha|} - \frac{2}{|\mathbf{r}_2 - \alpha|} + \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} + \mathbf{F}_{\rm DC}\cdot(\mathbf{r}_1 + \mathbf{r}_2 - 2\alpha), \quad (11)$$

where $\hat{T}$ is kinetic energy operator. The right-hand side of equation (11) is a periodic function of time which can be expanded as a Fourier series. If we retain in this expansion only the zero order harmonic, we shall obtain the so-called effective time-independent Hamiltonian. Clearly, such an approximation provides a valid picture if AC field frequency is considerably larger than the characteristic frequencies of the electron motion. In our problem the latter quantity can be roughly estimated as 20 eV (the distance from the ground to the first excited state). Then, for the AC field frequency of 111 eV which we consider in the paper, we can presumably use the described above approximation of the effective time-independent Hamiltonian. The DC field ionization in this picture can be viewed as a tunneling process in the effective potential of this Hamiltonian. The actual form of this potential may be quite complicated already for one-electron atoms [54]. As our results suggest, the tunneling rate in this potential may vary non-monotonously with the strength of the applied DC field. On the basis of this picture we may expect to observe similar behavior for all frequencies considerably larger than the characteristic frequency (20 eV) of the electron motion.

Another feature to notice for the ground state is that, as can be seen form Table 1, the level shifts due to AC and DC fields are opposite in signs so that for stronger AC fields the ground state level appears to be less shifted for a given DC field strength.

As far as the excited states are concerned, for the fixed AC field strength, the positions of the states $1s2s\ ^1$S and $1s2p\ ^1$P reveal a familiar pattern of the DC Stark effect for the closely spaced levels. For small values of the DC field strength we observe the typical avoided crossing behavior. With increase of the DC field, when DC Stark level shifts become larger than the energy separation between the levels, we observe a linear Stark effect. This is illustrated in Figure 2 for $F_{\rm AC} = 0.05$ a.u.

The overall shapes of the curves do not change appreciably with AC field strength, to save space we present the plots only for one value of the AC field strength (0.05 a.u. for the singlets and 0.1 a.u. for the triplets below).

The widths considered as functions of the DC field strength at a constant AC field strength also exhibit a typical DC Stark effect behavior growing monotonously with the DC field strength. As compared to the ground state, an order of magnitude weaker DC field is required to cause an appreciable change in the energy parameters of the excited states. This is not surprising given a much more diffuse orbitals of the excited states.

3.2 Triplet states

Calculation for the triplet states differed only in minor details of the composition of the basis. As for singlet states, to describe each Floquet block in system (7) we used the split-exponential Hylleraas type basis functions (8) with $L \leq 5$. As for singlets, each of the parameters a, b in equation (8) was allowed to assume two values: 1 and 0.5, chosen so to facilitate description of the states $1s2s$ and

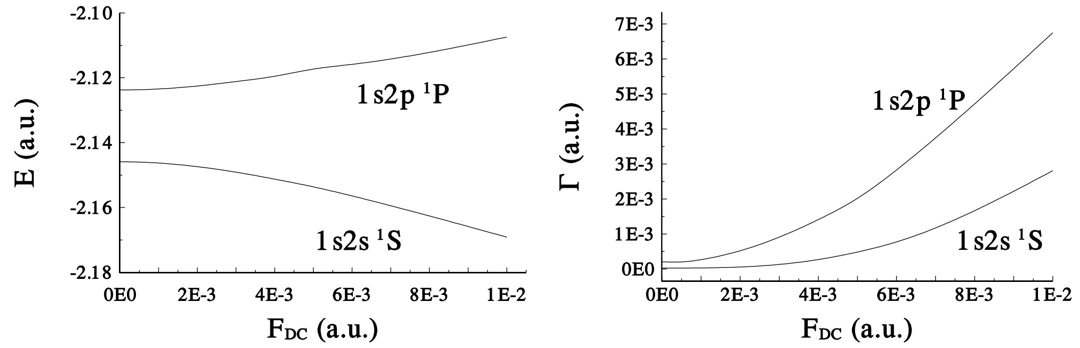

Fig. 2. Positions and widths (in a.u.) of the $1s2s$ ^{1}S and $1s2p$ ^{1}P states as functions of the DC field strength. The AC field frequency is $\omega = 111$ eV, strength $F_{\rm AC} = 0.05$ a.u.

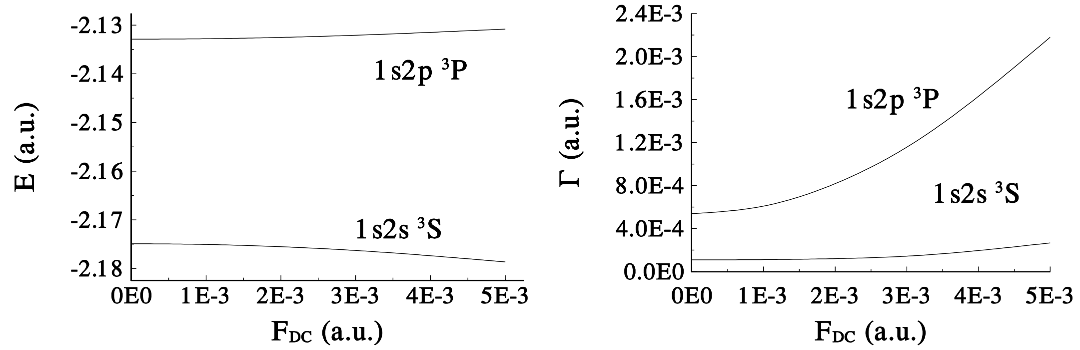

Fig. 3. Same as Figure 2 for the $1s2s$ ^{3}S and $1s2p$ ^{3}P states. The AC field frequency $\omega = 111$ eV, strength $F_{\rm AC} = 0.1$ a.u.

$1s2p$. For each of the Floquet blocks in set (7) we retain the basis functions of ^{3}S^e, ^{3}P^o, ^{3}D^e, ^{3}F^o, ^{3}G^e, ^{3}H^o symmetries for which the parameter $N_{\max}$ in (10) is equal to 9. Such a choice leads to the following composition of the basis set for each of the Floquet blocks: 220 ^{3}S^e, 336 ^{3}P^o, 78 ^{3}D^e, 70 ^{3}F^o, 47 ^{3}G^e and 30 ^{3}H^o basis functions, resulting in the total of 781 basis functions for each of the Floquet blocks. The results for the triplets reported below were obtained with the use of the $n = 0, \pm 1$ Floquet blocks in system (7). Overall dimension of the eigenvalue problem to be solved was 2343. To ensure that such a basis is adequate for our purposes, we repeated all the steps, described above for the singlets. For the field-free case we obtain the following results for the energies of the states of interest: -2.175229378 a.u. ($1s2s$ ^{3}S) and -2.133164357 a.u. ($1s2p$ ^{3}P). Comparing these values to the well-known nonrelativistic results [46] allows us to conclude that in the field-free case the basis described above allows to reach the accuracy of the order of 10^{-9} a.u. for the $1s2s$ ^{3}S state and 10^{-7} a.u. for the $1s2p$ ^{3}P state. Remaining checks (accuracy of the description of the ordinary DC Stark effect, stability with respect to the number of the Floquet blocks, etc.) were performed similarly to those described in the previous section. We will not, therefore, enter into the details, and quote only the final estimate of the accuracy to be of the order of 5×10^{-6} a.u. both for positions and widths. The numerical results for the triplet states are presented in Table 3, and Figure 3.

The energy separation of the triplet resonances is considerably larger than of the singlets. The avoided crossing behavior is, therefore, not so clearly pronounced as for singlets. The widths of the triplet states exhibit a monotonous growth with the DC field.

4 Conclusion

We performed a study of the ground and low lying excited states of the helium atom in the presence of the DC and AC electric fields. Our theoretical method relies on the recasting of the time-dependent Schrödinger equation into the Floquet representation with subsequent application of the complex rotation method [33]. To this theoretical foundation we added an efficient technical device — the Hylleraas basis set. Use of this set allowed us to make the solution of the present, rather complicated problem computationally feasible.

The study has been performed for singlet and triplet ground and low-lying excited states. Behavior of the positions and widths of the excited $1s2s$, $1s2p$ states is very similar to the picture observed for the ordinary DC Stark effect in two-electron systems. For the ground state, we noticed that until the magnitude of the applied DC field reaches approximately the magnitude of the AC field, the DC field has virtually no effect on the width. With some caution, the observed effect can be described as a decrease of the width with the DC field.

The technique used in the present work (a combination of the Hylleraas basis and the Floquet ansatz) allowed us to achieve quite a high accuracy in determining energy parameters of a rather complicated system: two-electron atom placed in external DC and AC fields. Use of Hylleraas basis allowed us to achieve this accuracy keeping the problem computationally manageable. The approach used is of a non-perturbative character and may be applied to the case of an atom in strong external fields. The algorithm of the calculation of the matrix elements used in the present paper allowed us to handle easily states of quite large angular momenta (states with total angular momentum $L \leq 5$ were included in the present work).

These features may be exploited further. They may allow us, for example, to describe another interesting phenomenon, the stabilization of two-electron systems in the presence of a very strong AC electric field [13]. For such strong fields (field intensities for stabilization to occur in He was found to be of the order of 2×10^{15} W cm^{-2} [55] one needs to include a large number of the Floquet blocks in system (7). Then, the ability of the Hylleraas basis to represent states of a system with relatively small number of basis functions may become quite useful.

The authors acknowledge support of the Australian Research Council in the form of Discovery grant DP0451211. Facilities of the Australian Partnership for Advanced Computing (APAC) were used.

Appendix

In this section we give some details of the calculation of the matrix elements of the Hamiltonian on the Hylleraas basis. We shall use the greek letters to designate the kets $|N, n_1, l_1, n_2, l_2; L\rangle$, given in the coordinate representation by equation (8).

It is easy to see that for the matrices **U** and **R** in equation (7) calculation of the matrix elements $\langle\alpha|\hat{C}|\beta\rangle$, (where $\hat{C}$ is either unit operator for the overlap matrix, or potential energy operator for the **U**-matrix), can be reduced to the calculation of the overlap matrix elements of the type $\langle\alpha|\beta'\rangle$, where the numbers N, n_j for the vector β', may differ from the corresponding numbers in the state β (e.g., for Coulomb repulsion term in the Hamiltonian $N^{\beta'} = N^{\beta} - 1$).

The calculation of the kinetic energy matrix elements can be performed quite analogously if one observes that the following easily derived identity holds for any (sufficiently smooth) function $f(\mathbf{r}_1, \mathbf{r}_2)$

$$\begin{aligned}(\Delta_1 + \Delta_2)|\mathbf{r}_1 - \mathbf{r}_2|^N f(\mathbf{r}_1, \mathbf{r}_2) = \\ \left(1 - \frac{N}{2}\right)|\mathbf{r}_1 - \mathbf{r}_2|^N (\Delta_1 + \Delta_2) f(\mathbf{r}_1, \mathbf{r}_2) \\ + 2N(N-2)|\mathbf{r}_1 - \mathbf{r}_2|^{N-2} f(\mathbf{r}_1, \mathbf{r}_2) \\ + \frac{N}{2}|\mathbf{r}_1 - \mathbf{r}_2|^{N-2}(\Delta_1 + \Delta_2)[(\mathbf{r}_1 - \mathbf{r}_2)^2 f(\mathbf{r}_1, \mathbf{r}_2)] \end{aligned} \quad (12)$$

where Δ is the Laplace operator. Using the fact that for our basis vectors $|N, n_1, l_1, n_2, l_2; L\rangle$ the function $f(\mathbf{r}_1, \mathbf{r}_2)$ is a product of two Slater-type functions, it is easy to see that equation (12) reduces the calculation of matrix elements of the energy operator in the basis of the vectors $|N, n_1, l_1, n_2, l_2; L\rangle$ to calculation of the basic matrix elements $\langle N_i, n_{1i}, l_{1i}, n_{2i}, l_{2i}; L|N'_j, n'_{1j}, l_{1j}, n'_{2j}, l_{2j}; L\rangle$. The latter can be calculated analytically with the help of the following expansion

$$|\mathbf{r}_1 - \mathbf{r}_2|^\lambda = r_>^\lambda \sum_{n=0}^{\infty} a_n(\alpha) P_n(\cos(\theta_{12})) \quad (13)$$

where $\alpha = r_</r_>$, $r_<$ and $r_>$ being as usual the larger and the smaller of the two coordinate vectors $\mathbf{r}_1$ and $\mathbf{r}_2$ respectively, and

$$\begin{aligned} a_n(\alpha) = 4^n \alpha^n \frac{\Gamma(n - \lambda/2)}{\Gamma(-\lambda/2)} \frac{n!}{(2n)!} \\ \times F(n - \lambda/2, -\lambda/2 - 1/2; n + 3/2; \alpha^2). \end{aligned} \quad (14)$$

In the last equation $F(n - \lambda/2, -\lambda/2 - 1/2; n + 3/2; \alpha^2)$ is a hypergeometric function.

With the help of expansion (13) the basic matrix elements are calculated much the same way as ordinary Slater integrals (to which they reduce of course if we put in Eq. (13) $\lambda = -1$). The calculation is much simplified by the fact that for all needed matrix elements the parameter λ in (13) is an integer satisfying $\lambda = N \geq -1$. Due to this fact the hypergeometric function in the equation (14) reduces to a polynomial, allowing thus to perform radial integrations analytically without lost of precision. Angular integrations are performed using standard angular momentum technique. Calculation of the dipole matrix elements in equation (7) proceeds analogously.

References

1. P.A.M. Gram, J.C. Pratt, M.A. Yates-Williams, H.C. Bryant, J. Donahue, H. Sharifian, H. Tootoonchi, Phys. Rev. Lett. **40**, 107 (1978)
2. S. Cohen, H.C. Bryant, C.J. Harvey, J.E. Stewart, K.B. Butterfield, D.A. Clark, J. Donahue, D.W. MacArthur, G. Comtet, W.W. Smith, Phys. Rev. A **36**, 4728 (1987)
3. A.R.P. Rau, H. Wong, Phys. Rev. A **37**, 632 (1988)
4. B. Gao, A.F. Starace, Phys. Rev. A **42**, 5580 (1990)
5. H. Bachau, F. Martin, J. Phys. B **29**, 1451 (1996)
6. T.K. Fang, Y.K. Ho, Phys. Rev. A **60**, 2145 (1999)
7. K.T. Chang, T.K. Fang, Y.K. Ho, J. Phys. B **34**, 165 (2001)
8. T.K. Fang, K.T. Chang, J. Phys. B **34**, 1245 (2001)
9. J.R. Harries, J.P. Sullivan, J.B. Sternberg, S. Obara, T. Suzuki, P. Hammond, J. Bozek, N. Berrah, M. Halka, Y. Azuma, Phys. Rev. Lett. **90**, 133002 (2003)
10. X.M. Tong, C.D. Lin, Phys. Rev. Lett. **92**, 223003 (2004)
11. W.P. Reinhardt, Ann. Rev. Phys. Chem. **33**, 223 (1982)
12. A. Buchleitner, B. Gremaud, D. Delande, J. Phys. B **27**, 2663 (1994)
13. M. Gavrila, J. Phys. B **35**, R147 (2002)
14. P.G. Burke, P. Francken, C.J. Joachain, J. Phys. B **24**, 751 (1991)
15. P.G. Burke, V.M. Burke, J. Phys. B **30**, L383 (1997)
16. J. Purvis, M. Dörr, M. Terao-Dunseath, C.J. Joachain, P.G. Burke, C.J. Noble, Phys. Rev. Lett. **71**, 3943 (1993)

17. M. Dorr, J. Purvis, M. Terao-Dunseath, P.G. Burke, C.J. Joachain, C.J. Noble, J. Phys. B **28**, 4481 (1995)
18. J. Colgan, D.H. Glass, K. Higgins, P.G. Burke, J. Phys. B **34**, 2089 (2001)
19. P. Lambropoulos, P. Maragakis, J. Zhang, Phys. Rep. **305**, 203 (1999)
20. A. Saenz, Phys. Rev. A **66**, 063407 (2002)
21. A. Srinzi, B. Piraux, Phys. Rev. A **58**, 1310 (1998)
22. J. Caillat, J. Zanghellini, M. Kitzler, O. Koch, W. Kreuzer, A. Srinzi, Phys. Rev. A **71**, 012712 (2005)
23. C.A. Nicolaides, T. Mercouris, Chem. Phys. Lett. **159**, 45 (1989)
24. S.I. Themelis, T. Mercouris, C. A. Nicolaides, Phys. Rev. A **61**, 024101 (1999)
25. C.A. Nicolaides S. I. Themelis, Phys. Rev. A **47**, 3122 (1993)
26. C. Cerjan, W.P. Reinhardt, J. Avron, J. Phys. B **11**, L201 (1978)
27. J. Avron, I. Herbst, Commun. Math. Phys. **52**, 239 (1977)
28. I. Herbst, Commun. Math. Phys. **64**, 279 (1979)
29. Y.K. Ho, A.K. Bhatia, Phys. Rev. A **44**, 2895 (1991)
30. Y.K. Ho, J. Callaway, Phys. Rev. A **50**, 4941 (1994)
31. A. Saenz, J. Phys. B **35**, 4829 (2002)
32. W.P. Reinhardt, S. Han, Int. J. Quant. Chem. **57**, 327 (1996)
33. S.I. Chu, W.P. Reinhardt, Phys. Rev. Lett. **39**, 1195 (1977)
34. A. Buchleitner, D. Delande, J. Gay, J. Opt. Soc. Am. B **12**, 505 (1995)
35. R.M. Potvliege, Comp. Phys. Comm. **114**, 42 (1998)
36. S.-I. Chu, D.A. Telnov, Phys. Rep. **390**, 1 (2004)
37. G.W.F. Drake, Phys. Scripta T **83**, 83 (1999)
38. B. Yang, M. Pont, R. Shakeshaft, E. van Duijn, B. Piraux, Phys. Rev. A **56**, 4946 (1997)
39. I.A. Ivanov, A.S. Kheifets, Eur. Phys. J. D, e-print `10.1140/epjd/e2005-00334-y`
40. J.H. Shirley, Phys. Rev. **138**, B979 (1965)
41. D.R. Dion, J.O. Hirschfelder, Adv. Chem. Phys. **35**, 265 (1976)
42. B.R. Johnson, W.P. Reinhardt, Phys. Rev. A **28**, 1930 (1983)
43. Y.K. Ho, Phys. Rep. **99**, 1 (1983)
44. B.R. Junker, Adv. At. Mol. Phys. **18**, 208 (1982)
45. I.A. Ivanov, Y.K. Ho, Phys. Rev. A **69**, 023407 (2004)
46. C.L. Pekeris, Phys. Rep. **115**, 1216 (1959)
47. J.A.R. Samson, Z.X. He, L. Yin, G.N. Haddad, J. Phys. B **27**, 887 (1994)
48. C.A. Nicolaides, S.I. Themelis, J. Phys. B **26**, L387 (1993)
49. I.A. Ivanov, Y.K. Ho, Phys. Rev. A **63**, 062503 (2001)
50. L.V. Keldysh, Sov. Phys.-JETP **47**, 1495 (1964)
51. H.A. Kramers, *Collected Scientific Papers* (North Holland, Amsterdam, 1956)
52. W.C. Henneberger, Phys. Rev. Lett. **21**, 838 (1968)
53. I. Gilary, N. Moiseev, Phys. Rev. A **66**, 063415 (2002)
54. N.B. Delone, V.P. Krainov, *Multiphoton Processes in Atoms* (Springer-Verlag, Berlin, 1994)
55. N. Moiseev, L.S. Cederbaum, J. Phys. B **32**, L279 (1999)