

# Helium atom in the monochromatic electromagnetic field

## A Hylleraas basis treatment

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**Abstract.** We apply a non-perturbative procedure for the calculation of the total photoionization cross-section of two-electron atomic systems. The procedure is based on the Floquet-Fourier representation of the time-dependent Schrödinger equation. With the use of the Hylleraas-type basis functions, the total photoionization cross-sections obtained are within the accuracy of a fraction of a percent, which, we believe, is the most accurate estimate for the cross-sections available. The total photoionization cross-sections for neutral helium deviate notably from the benchmark experimental data [J.A.R. Samson et al., J. Phys. B **27**, 887 (1994)].

**PACS.** 32.80.Fb Photoionization of atoms and ions – 32.80.-t Photon interactions with atoms – 32.80.Rm Multiphoton ionization and excitation to highly excited states (e.g., Rydberg states)

## 1 Introduction

Photoionization of two-electron atoms has been studied theoretically by different authors starting from the pioneering paper [2]. Review of early literature on this subject can be found in [3]. Subsequently, a large number of computations of helium photoionization cross-sections was reported [4–7]. These calculations produced a collection of results varying typically by 5% from each other. On the experimental side, the benchmark set of data was reported by Samson and co-workers [1,8]. Agreement between the theoretical and experimental data was within the same margin of 5%. In the following years, the theoretical interest shifted towards calculation of differential characteristics of the photoionization process and to studies of double photoionization. Here, several approaches have been advocated including the many-body perturbation theory [7,9], convergent close-coupling method [10,11], many electron many photon approach [12,13], time-dependent close-coupling method [14–16], *R*-matrix approach [17,18], and methods based on the computation of the dipole response function [19] or *B*-spline implementations of the exterior complex scaling [20,21].

Due to this shift of focus, there have been no further attempts to produce a consistent set of photoionization cross-sections of He with an accuracy of better than several percent. In the meantime, accurate helium photoionization cross-sections would be highly desirable due to importance of He in astrophysics and its use as a standard gas in determination of the photoionization cross-sections of other atomic and molecular species.

In the present paper we report a calculation of the total photo-ionization cross-section from the ground state of helium, which we believe provides results accurate to within a fraction of a percent. We were able to attain this level of accuracy by reformulating the description of the photoionization process in terms akin to those used in the bound-state calculations, and by borrowing one important tool used in the bound-state calculations, namely the Hylleraas basis set. It is use of this tool which allows unprecedented accuracy of the bound-state calculations in few-electron systems. Use of this tool allows also, as we hope to demonstrate, achieve quite high accuracy in the photoionization calculations, even in the regime of relatively high intensities of the applied electromagnetic field.

To achieve this goal we combine the so-called complex rotation method (CRM) and the Hylleraas basis technique.

There is a long history of using the CRM method in the photoionization calculations. One way of calculating the photoionization cross-section is to combine the CRM technique with the perturbation theory with respect to interaction of the atom with the electromagnetic field. In such a perturbation theory, the CRM provides the basis of the field-free atomic states. It was demonstrated [22] that relying on the spectrum of the CRM eigenvalues, one can construct a representation of the complete Green's function of the atom. This, in turn, allows to write down a convenient representation for the projection operator corresponding to the continuous spectrum of the atom [23]. Using this projection operator, one can compute probabilities of transitions into continuum under the action of some perturbation, in particular, the interaction of the

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atom with the electromagnetic field. Calculations of total photoionization cross-sections of the helium atom, based on this technique, have been reported in [24,25].

Alternative, completely nonperturbative approach to the description of EM-radiation-atom interaction, has been proposed in reference [26] which also relies on the ideas of the CRM technique. This approach becomes feasible in the so-called Floquet-Fourier representation of the time-dependent Schrödinger equation [27]. This representation allows to reduce the problem of solving the time-dependent Schrödinger equation to a somewhat simpler task of finding solution of a set of differential equations. The CRM is a convenient tool which allows to solve this problem efficiently. Thus, starting from the pioneering work [26], the combination of these methods has been used in a number of works devoted to the study of atom-EM radiation interaction [28–30].

The key ingredient of the present work, which distinguishes it from previous implementations of the Floquet-CRM method, is the use of the Hylleraas basis functions. This basis has long been used in variational-type calculations of bound states. An excellent review of applications of the Hylleraas basis to calculations of energies of two-electron atoms is given in reference [31]. A well-known trademark of the Hylleraas basis set is a very high accuracy, which use of this basis allows to reach.

In the present paper, we show that the same high accuracy which is achieved for field-free atomic states can also be attained when the atom is placed in a monochromatic electromagnetic field. In particular, the total photoionization cross-sections can be calculated with an unprecedented accuracy of the order of a fraction of a percent.

Thus generated cross-sections were compared with the experimental results [1]. Within the present accuracy, we discovered a systematic deviation from the experiment, especially in the region close to double ionization threshold at the photon energies of  $\sim 80$  eV. This deviation was confirmed by comparison with earlier results produced by the convergent close-coupling (CCC) method [32].

The true potential of the present approach is realized in the strong field regime where the perturbation theory fails. As demonstrated below, the Floquet-Fourier-Hylleraas ansatz produces very accurate results in this regime as well.

## 2 Theory

### 2.1 General theory

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

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

where we adopt the length gauge to describe interaction of atom and the field, and  $\mathbf{D} = \mathbf{r}_1 + \mathbf{r}_2$ . Unless stated otherwise, the atomic units are used throughout the paper.

We shall also assume that the field is directed along the  $z$ -axis.

We write the solution of the time-dependent Schrödinger equation (TDSE) using the Floquet-Fourier ansatz [26,27,33,34].

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

By substituting this expression into the TDSE and equating coefficients with  $e^{-iEt - im\omega t}$ , we obtain a chain of coupled equations for the Floquet-Fourier coefficients  $u_n$ :

$$(E - \hat{T} - \hat{U} + n\omega)u_n = \frac{\mathbf{F} \cdot \mathbf{D}}{2}(u_{n-1} + u_{n+1}), \quad n = 0, \pm 1, \dots, \quad (3)$$

where  $E$ ,  $\hat{T}$  and  $\hat{U}$  stand, respectively, for the quasienergy, and operators of kinetic and potential energy.

This set of equations can be solved with the help of the CRM procedure [35–40]. Formally, the CRM can be described as a complex transformation of radial variables  $r_i \rightarrow r_i e^{i\theta}$ , where  $\theta$  is the rotation angle, the sole parameter defining the transformation.

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

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

where  $n = 0, \pm 1, \dots$

According to the general theory of CRM [35–38], the set of equation (4) can be solved by means of variational techniques if the rotation angle  $\theta$  is properly chosen.

As usual in the variational calculations, 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  $n$ th 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:

$$\left( (E + n\omega)R_{n_1 k_1}^{nk} - T_{n_1 k_1}^{nk} e^{-2i\theta} - U_{n_1 k_1}^{nk} e^{-i\theta} \right) c_{nk} = \sum_{n_2 = n \pm 1} V_{n_1 k_1}^{n_2 k} \frac{e^{i\theta}}{2} c_{n_2 k}, \quad (5)$$

where it is understood that summation is carried over the repeated  $k$ -index. Here  $\hat{V} = \mathbf{F} \cdot \mathbf{D}$ , and  $R$ ,  $T$  and  $U$  stand for the overlap, kinetic energy and potential energy matrices, respectively.

One should say here a few words about the choice of the basis allowed by the structure of the system (5). Suppose first, that in each of the subspaces, corresponding to different Floquet blocks, we chose some complete set of functions, such that for any  $u_n$  in equation (4) we had:  $u_n = \sum c_{nm}|n, m\rangle$ . Let the set of  $|n, m\rangle$ 's be the same for all Floquet subspaces. Then, if we have retained  $N$  Floquet blocks in the system (4) and keep  $M$  terms in

the expansion for each  $u_n$  in equation (4) we have altogether  $NM$  unknowns  $c_{nm}$  in the system (4). To get a correctly posed eigenvalue problem, we should have the same number of equations. This number is provided by projecting each of the equations (4) on one of the  $|n, m\rangle$ 's with  $m = 1 \dots M$ . This way of reducing the set of equations (4) to the form of matrix eigenvalue problem is correct, but too general for our purposes. It can be seen, that one can reduce considerably the resulting dimension of the matrix eigenvalue problem by using certain symmetry properties of the system equation (4). It is easy to see that this system allows the following class of solutions:  $u_n$ 's with even  $n$  are of even parity, while  $u_n$ 's with odd  $n$  are of odd parity. Parity here is understood with respect to the spatial inversion. Of course, there is a class of solutions with the opposite property:  $u_n$ 's with even  $n$  are of odd parity, while  $u_n$ 's with odd  $n$  are of even parity. The solution we are looking for (which is to describe behavior of the even  $^1S^e$  state of helium) evidently belongs to the first class. We can therefore, choose the basis set as follows.

Instead of choosing the same set  $|n, m\rangle$  for each Floquet block, we choose two sets: a set  $|n_{\text{even}}, m\rangle$ , consisting of basis functions of even parity, is used as a basis to represent  $u_n$ 's with even  $n$ 's. Another set  $|n_{\text{odd}}, m\rangle$ , composed of odd parity functions is used as a basis to represent  $u_n$ 's with odd  $n$ 's. Suppose that in the expansions of  $u_n$ 's with even  $n$ 's we retain  $M_{\text{even}}$  terms, and in the expansions of  $u_n$ 's with odd  $n$ 's— $M_{\text{odd}}$  terms. Let the number of Floquet blocks with even and odd  $n$ 's be respectively  $N_{\text{even}}$  and  $N_{\text{odd}}$ . Then we have  $N_{\text{even}}M_{\text{even}} + N_{\text{odd}}M_{\text{odd}}$  unknown coefficients  $c_{nm}$ . We obtain the same number of equations by projecting equation (4) on  $|n_{\text{even}}, m\rangle$ ,  $m = 1 \dots M_{\text{even}}$  for even  $n$  and on  $|n_{\text{odd}}, m\rangle$ ,  $m = 1 \dots M_{\text{odd}}$  for odd  $n$ . Projection of equations with even  $n$  on the  $|n_{\text{odd}}, m\rangle$  and of equations with odd  $n$  on the  $|n_{\text{even}}, m\rangle$  gives identically zero and does not add new equations. More details about the basis functions  $|n_{\text{even}}, m\rangle$  and  $|n_{\text{odd}}, m\rangle$  is given below.

According to the general theory of CRM, some of the energy values (generally complex) for which system (5) has a solution are related to the position and width of the resonance state via  $E = E_r - i\Gamma/2$ , where  $E_r$  is position of the resonance and  $\Gamma$  its width. This leads one to solving a generalized eigenvalue problem. Efficiency of finding eigenvalues of such a problem depends crucially on the choice of the basis used to represent the matrices in equation (5). So far, the development has been fairly general and well-known, following, e.g., the ideas presented in [26]. We introduce now a major technical improvement, consisting in the choice of the basis functions.

## 2.2 Basis set

The basis set used in the present paper was constructed from the Hylleraas type functions:

$$g_{n_1, n_2, N}(\mathbf{r}_1, \mathbf{r}_2) = r_1^{n_1} r_2^{n_2} |\mathbf{r}_1 - \mathbf{r}_2|^N e^{-ar_1 - br_2} |l_1(1)l_2(2)L\rangle, \quad (6)$$

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

$$|l_1(1)l_2(2)L\rangle = \sum_{m_1 m_2} C_{l_1 m_1 l_2 m_2}^{LM} Y_{l_1 m_1}(\mathbf{n}_1) Y_{l_2 m_2}(\mathbf{n}_2), \quad (7)$$

represents two angular momenta  $l_1, l_2$  coupled to a state with a total angular momentum  $L$ . The basis functions (6) must be properly symmetrized with respect to exchange of the electron coordinates. When choosing parameters in equation (6), we followed the following rule of thumb [31, 41]. All the basis functions with the parameters satisfying:

$$n_1 + n_2 + N < N_{\text{max}} \quad (8)$$

were included in the calculation (this inequality defines the so-called Pekeris shell). The parameter  $N_{\text{max}}$  determines the overall size of the basis. There is also a semiempirical rule for choosing angular momenta  $l_1, l_2$  in equation (6). Thus, for states of 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.

## 3 Numerical results

### 3.1 Field-free case

In the present work, our main goal is to obtain accurate photoionization cross-sections from the ground state of neutral helium for not very large electromagnetic field intensities. Accordingly, our main interest is focused on the states of S and P symmetries. Therefore, our first goal is to choose such a basis that solution of the eigenvalue problem (5) yields accurate energies for the ground  $^1S$  and first excited  $^1P^0$  state of the helium atom in the absence of the field.

This goal was achieved as follows. We chose parameters  $N_{\text{max}} = 18$ ,  $a = b = 2$  for the S-states and  $N_{\text{max}} = 12$ ,  $a, b = 1, 2$  for the P-states. The reason for enlarging the basis set for the excited P-states is that the electrons in such states are generally on different distances from the nucleus. This choice combined with restriction on angular momenta, given by equation (8) resulted in  $N_S = 372$  basis functions for the S-states and  $N_P = 660$  basis functions for the P-states.

The next step was to solve the generalized eigenvalue problem for the field-free case. In equation (5) we put  $F = 0$ ,  $\omega = 0$ , and limited ourselves to the blocks with  $n = 0$ ,  $n = \pm 1$ , the  $n = 0$  block being composed of the states of  $^1S^e$  symmetry, and  $n = \pm 1$  blocks composed of the states of  $^1P^0$  symmetry. All the numerical results reported below were obtained using the quadruple precision arithmetic.

We note, that in the presence of the weak electromagnetic field, account of the blocks with  $n = \pm 1$  corresponds to absorption and emission of one photon. We shall use this fact below to extract the photoionization cross-section from our calculation. For the moment, we are concerned

with testing the accuracy of our basis. Diagonalization of the eigenvalue problem (5) with  $F = 0$ ,  $\omega = 0$  in the basis described above produced the following results for the complex energies:  $E = -2.903724384 + i 1.3 \times 10^{-8}$  (the ground state) and  $E = -2.123843094 + i 7.6 \times 10^{-9}$  ( $1s2p^1P^0$  state). A small imaginary part which, in the absence of the field, should of course be zero could be taken as an indication of an accuracy of our basis set. Either this criteria or a direct comparison with the well-known results of highly accurate calculations [31] shows that we have achieved an accuracy of the order of  $10^{-8}$  a.u. This accuracy, as will be demonstrated below, is sufficient to obtain the photoionization cross-sections with at least three significant figures.

### 3.2 Total photoionization cross-sections

To calculate the total photoionization cross-sections we adopted the following strategy. The eigenvalue problem (5) was solved with the Floquet blocks  $n = 0, \pm 1$  retained, the composition of each block was the same as described above for the field-free case. Diagonalization of the eigenvalue problem (5) produced energy shift and total width for the ground state. By definition, the photoionization cross-section from this state is related to the total width  $\Gamma$  via

$$\sigma = \lim_{F \rightarrow 0} 8\pi\alpha\Gamma\omega/F^2, \quad (9)$$

where  $F$  is field strength,  $\omega$  its frequency,  $\alpha$  is the fine structure constant. We need therefore to extract from our calculation the coefficient with  $F^2$  in the asymptotic law defining the weak-field behavior of the width:

$$\Gamma(F) = \Gamma_0 F^2 + \Gamma_1 F^3 + \dots \quad (10)$$

To implement this strategy, we need an extrapolation procedure since the calculation based on the system (5) is performed for a non-zero field strength. Although finite, this field strength should not be too small to compute  $\Gamma$  with sufficient accuracy.

The issue of accuracy can be addressed as usual in variational-type calculations, by merely increasing the basis size and verifying that the results do not change appreciably. Such a test was performed for a photon energy  $\omega = 80$  eV and a field strength  $F = 0.1$  a.u. by varying the parameter  $N_{\max}$  in equation (8) for the S and P states. The diagonalization of the problem (5) was performed with the Floquet blocks  $n = 0, \pm 1$  retained. All the remaining details of the basis (nonlinear parameters, etc.) were the same as in the field-free case reported above. The calculation was performed for the value of the rotation angle  $\theta = 0.3$ .

The test results are presented in Table 1. One can observe that, just as in the field-free case, the accuracy is on the level of  $10^{-8}$  a.u., which implies that  $\Gamma$  has at least four significant digits in this interval of field strengths.

Another check of the accuracy can be obtained by studying dependence of the resonance parameters upon the rotation angle  $\theta$ . We repeated the calculation described above (with  $N_{\max}^S = 18$ ,  $N_{\max}^P = 12$ ) for various

**Table 1.** Results for the ground state eigenvalue of problem (5) as functions of parameters  $N_{\max}$  in equation (8),  $\omega = 80$  eV,  $F = 0.1$  a.u.

$N_{\max}^S$	$N_{\max}^P$	Total dimension of the eigenvalue problem (5)	Re $E$ (a.u.)	$\Gamma$ (a.u.)
17	11	1300	-2.90307660	0.000487738
18	12	1692	-2.90307661	0.000487698
19	13	2204	-2.90307659	0.000487689

**Table 2.** Dependence of the ground state eigenvalue of problem (5) ( $N_{\max}^S = 18$ ,  $N_{\max}^P = 12$ ) as function of the rotation angle  $\theta$ ,  $F = 0.1$  a.u.

$\theta$	Re $E$ (a.u.)		$\Gamma$ (a.u.)	
	$w = 80$ eV		$w = 111$ eV	
0.20	-2.90307627	0.000488071	-2.90338566	0.000146997
0.25	-2.90307654	0.000487729	-2.90338579	0.000147052
0.30	-2.90307661	0.000487698	-2.90338581	0.000147074
0.35	-2.90307660	0.000487683	-2.90338582	0.000147085
0.40	-2.90307660	0.000487689	-2.90338582	0.000147094

values of  $\theta$  in the interval  $\theta \in [0.20, 0.40]$ . Results are presented in Table 2 for the photon frequencies of 80 eV and 111 eV and for the field strength of 0.1 a.u.

As one can see, in the vicinity of  $\theta = 0.30$  variation of the results is within the bounds of accuracy established above, confirming thus this accuracy estimate and the choice of the rotation angle ( $\theta = 0.30$ ) for which all the subsequent calculations have been performed.

The issue of the stability of the results with respect to the number of the Floquet blocks included in diagonalization of (5) is addressed in the next section where we consider effects of going beyond the first order perturbation theory. We shall say in advance that, for the field strengths considered, inclusion of the Floquet blocks with  $n = \pm 2$  in diagonalization of (5) does not alter the numerical accuracy appreciably.

As to the extrapolation procedure needed to extract the coefficient  $\Gamma_0$  in equation (10), we chose a scheme based on the three-point Lagrange formula. For each frequency reported below, we performed calculations for the field strengths  $F = 0.07, 0.1, 0.13$  a.u. We also used a mid size basis set with  $N_{\max}^S = 18$ ,  $N_{\max}^P = 12$ , Floquet blocks with  $n = 0, \pm 1$ , all other details of the basis being the same as in the field-free case above. Results of this calculation and extrapolation procedure are shown in Table 3.

Using an estimate for the remainder of the series (10), it is a simple matter to verify that for the field strengths considered the possible relative error introduced by the extrapolation of  $\Gamma/F^2$  is on the order of 0.1%. Hence, at least three digits in our result for the extrapolated ratio  $\Gamma/F^2$  and the cross-sections reported below must be reliable. This level of accuracy can easily be improved by merely going to extrapolation schemes of higher order and computing  $\Gamma$  for more field values.

**Table 3.** Extrapolation of the  $\Gamma$ 's to the zero-field limit.

$\omega$ (eV)	$\Gamma/F^2$ (a.u.)			
	$F = 0.07$ a.u.	$F = 0.1$ a.u.	$F = 0.13$ a.u.	$F = 0$ (Extrapolation)
40	0.4208622	0.4201601	0.4192063	0.4215215
80	0.0488002	0.0487698	0.0487239	0.0488112
85	0.0392854	0.0392618	0.0392330	0.0393202
91	0.0306858	0.0306720	0.0306524	0.0306961
95	0.0262180	0.0262082	0.0261936	0.0262224
111	0.0147116	0.0147084	0.0147033	0.0147116
205	0.0013719	0.0013726	0.0013729	0.0013687

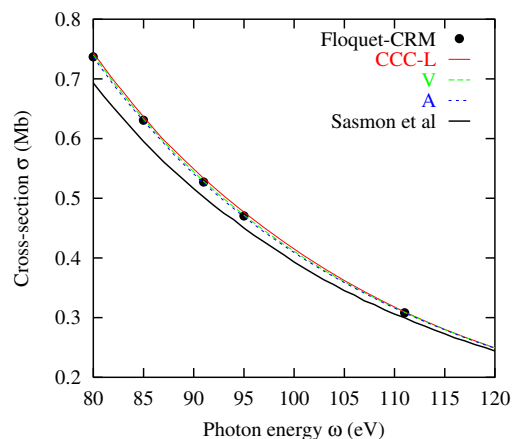
**Table 4.** Comparison of the present results and other theoretical and experimental data for the total photoionization cross-section (in Mb).

$\omega$ eV	Present	CCC		Experiment		Compilation [43]
		L	V	[1]	[42]	
40	3.1822	3.188	3.178	3.16	3.183	3.190
80	0.7369	0.7432	0.7403	0.693	0.715	0.702
85	0.6308	0.6364	0.6327	0.595	0.611	
91	0.5272	0.5333	0.5284	0.502	0.509	
95	0.4701	0.4765	0.4717	0.450	0.452	
111	0.3082	0.3097	0.3089	0.300		
205	0.0529	0.0533	0.0534	0.0510		0.0533

In Table 4 we present our results for the cross-sections based on formula (9) in which we fed the extrapolated ratios from the last column of Table 3. Along with our data, we present the experimental results of Samson and co-workers [1,8,42] as well as earlier theoretical results from [32] and compilation [43]. Graphical illustration of the present results, theoretical results obtained by means of the CCC method, and the experimental data [1] is given in Figure 1.

For the photon energy of 40 eV, we also compare our results with a highly accurate multichannel calculation of [44]. Using a combination of configuration interaction and close-coupling techniques, these authors obtained the following values for the total single ionization cross-section: 3.18173 Mb (length gauge), 3.18129 Mb (velocity gauge) and 3.18056 Mb (acceleration gauge). Variation of these results with the gauge is on the order of  $5 \times 10^{-4}$  Mb which can be used as a measure of the accuracy of their calculation. These results are to be compared with our cross-section of 3.1822 Mb which is within the limits of  $5 \times 10^{-4}$  Mb from the length gauge of [44]. We may therefore conclude that we achieved at least the same level of accuracy in the description of the single-electron ionization as was reported in the work [44]. Our calculation, however, covers the region of larger frequencies, where the double electron photoionization channel is open.

The deviation of the present data and the experimental data [1] reaches 6 percent for  $\omega = 80$  eV. This fact deserves some attention, we believe, since helium often serves

**Fig. 1.** Total photo-ionization cross-section from the ground state of helium. Present Floquet-CRM results are indicated by dots. The CCC calculation in the length, velocity and acceleration gauges are shown by solid (red), dashed (green) and dotted (blue) lines, respectively. Experimental data of Samson et al. [1] are displayed by a thick solid line. A color version of the figures is available in electronic form at <http://www.eurphysj.org>.

as a “standard” in photoionization cross-section measurements, and, therefore, precise knowledge of parameters characterizing photoionization in helium is of considerable practical importance. Agreement between the present calculation and that of the CCC is much better, difference of the results of two approaches not exceeding 1%. The accuracy of the CCC result is hard to estimate directly as this method relies on the numerical solution of a set of close-coupling equations. The only implicit indication is the difference between the cross-sections calculated using length (L) and velocity (V) gauges to describe atom-EM radiation interaction. This difference is typically 1–2%. Thus, the deviation of the present calculation with the CCC is more likely to be the problem of the latter as the former is believed to be much more accurate. As data from Table 4 show, the present results which rely on the length-form representation of the atom-EM interaction agree somewhat better with the velocity-form CCC results than with the length-form CCC data. We would be hesitant to ascribe any physical significance to this fact. Different gauges put different emphasis on the wavefunction to describe accurately photoionization process. In particular, the length gauge puts more emphasis on the atomic wave-functions at large distances which contribute little to the total energy of the bound state and therefore are poorly represented in variational calculations. Therefore the length gauge CCC results may be slightly less accurate than the velocity gauge results.

In the paper [21] the authors compared their total photoionization cross-section with the experimental data [1]. They concluded that the agreement between theory and experiment was excellent in the whole energy range, except in the vicinity of the resonance peaks due to the limited energy resolution of the experiment. This agreement was also categorized as very good in the region where

the double ionization continuum was open. As the results of reference [21] were presented graphically, it is hard to make a quantitative comparison between theory and experiment. Visual magnification of their cross-section plot (Fig. 6) reveals that the calculated cross-section is somewhat larger than the measured one close to double ionization threshold. For larger photon energies, our results are in good agreement with the results obtained by [43] who used large-energy asymptotic expansions for the cross-sections.

### 3.3 Extended calculation

We now turn to extended calculations with inclusion of a larger number of the Floquet blocks  $n = 0, \pm 1, \pm 2$  in equation (5). The aim of this calculation is two-fold. First, we shall confirm the stated accuracy of the present weak field results, showing that it is not effected by the number of the Floquet blocks retained in the calculation. Second, we report some preliminary results concerning behavior of the widths parameter in stronger fields where inclusion of a larger number of the Floquet blocks becomes essential due to the non-perturbative nature of the processes involved.

The basis for the extended calculations was constructed as follows. As we discussed above, the basis subset, spanning each Floquet block in system (5), can be chosen to consist of the functions of a given parity, two adjacent blocks having opposite parities. Thus, in the low-field calculations described above, the block  $n = 0$  was composed of even basis functions while two blocks with  $n = \pm 1$  contained odd basis functions. Inclusion of the blocks with  $n = \pm 2$  is, therefore, equivalent to adding more even basis functions. We did it in the following way. In addition to the  $^1S^e$  states we previously had in the  $n = 0$  block, the states of the  $^1D^e$  symmetry were included in the calculation. We need not consider states of the  $^1P^e$  symmetry. Indeed, in our problem, the  $z$ -projection of the total angular momentum  $M$  is a conserved quantity. In the present paper we are interested only in the manifold of states with  $M = 0$ . For  $M = 0$  all matrix elements  $\langle P^e M | D_z | P^0 M \rangle$  vanish. The blocks with  $n = 0$  and  $n = \pm 2$  had the following composition:  $N_{\max} = 18$  for the  $^1S^e$ -basis functions,  $N_{\max} = 8$  for the  $^1D^e$ -basis functions. As before, the blocks with  $n = \pm 1$  were composed of basis functions of  $^1P^0$ -symmetry with  $N_{\max} = 12$ . Thus, the basis set is considerably enlarged comparing to the one used in the previous section. With this choice of parameters  $N_{\max}$ , the overall dimension of the eigenvalue problem (5) was 2607. Results produced for the ground state of He by diagonalizing this eigenvalue problem are shown in Table 5. Comparison of the results given in Table 5 supports the assertion we made in the previous section as to the accuracy of our results for the widths. As one can see, for the field strengths  $F \approx 0.1$  a.u., inclusion of the additional Floquet blocks and basis states of symmetries other than S and P produces relative variations in the widths of the order of 0.01 percent. This means that for

**Table 5.** Results of the calculation with Floquet blocks  $n = 0, \pm 1, \pm 2$  included in the system (5).

$F$ (a.u.)	$\omega = 111$ eV		$\omega = 205$ eV	
	Re $E$ (a.u.)	$\Gamma/F^2$ (a.u.)	Re $E$ (a.u.)	$\Gamma/F^2$ (a.u.)
0.10	-2.90338569	0.014714	-2.90362976	0.0013734
0.13	-2.90315198	0.014715	-2.90356447	0.0013739
0.20	-2.90236955	0.014715	-2.90334589	0.0013743
0.50	-2.89525524	0.014706	-2.90135842	0.0013745
1.0	-2.86985102	0.014665	-2.89426254	0.0013701

such field values we are still within the domain of the validity of the perturbation expansion. For the frequencies presented in the table, the domain of the perturbation theory actually extends quite far in the region of large field strengths. As one can see from Table 5, the ratio  $\Gamma/F^2$  starts changing in an appreciable manner only for field strengths as large as  $F \approx 1$  a.u., which is where a truly non-perturbative regime starts. We cannot claim, of course, that the estimates of accuracy we made above are valid for the field strengths as large as  $F \approx 1$  a.u. These estimates were restricted to a region of the field strengths  $F \approx 0.1$  a.u. The entries for the field strength  $F = 1$  a.u. in Table 5 are intended rather as a demonstration of the fact that the ratio  $\Gamma/F^2$  starts changing appreciably only for field strengths as large as  $F \approx 1$  a.u. A proper accuracy estimate pertaining for this region of the much larger fields would require repeating all the steps we made above for smaller fields region (stability with respect to variation of the basis composition, rotation angle, number of the Floquet blocks, etc.). As we mentioned above the results presented in this section bear a preliminary character. We shall not, therefore, perform a thorough study to obtain an accuracy estimate pertaining for the region of the strong fields  $F \approx 1$  a.u. An indication of the possible accuracy our data for  $F \approx 1$  a.u. may have, can be obtained by changing the composition of the basis. We performed such a check, repeating a calculation described above with enlarged basis set. More specifically, we added more basis functions of the  $^1D^e$ -symmetry. For this calculation the  $n = 0, n = \pm 2$  blocks contained  $^1D^e$  basis functions with  $N_{\max} = 10$ . Correspondingly, the total number of the basis functions of  $^1D^e$  symmetry becomes 134 in each block with even  $n$  (comparing to 57 for the calculation with  $N_{\max} = 8$  reported in Tab. 5). Overall dimension of the eigenvalue problem (5) becomes 2838. This calculation produces the following results for the resonance parameters of the ground state for the photon frequency of 111 eV:  $E = -2.89525515$  a.u. (level position) and  $\Gamma/F^2 = 0.0147077$  a.u. (level width) for  $F = 0.5$  a.u., and  $E = -2.86984886$  a.u. and  $\Gamma/F^2 = 0.014672$  a.u. for  $F = 1.0$  a.u. Comparison of these numbers with the corresponding entries from Table 5 shows that even for the field strengths as large as  $F = 1.0$  a.u. we seem to have achieved a convergence with respect to the variation of the composition of the basis. This circumstance may be a consequence of the fact that a comparatively large frequency considered

diminishes the effect of the EM field-atom interaction. We emphasize, that this comparison should serve only as a rough guide, no reliable error bounds for the high fields (of the order of 1 a.u.) can be drawn from it.

## 4 Conclusion

We performed a calculation of the total photoionization cross-sections from the ground state of helium. We employed a theoretical procedure based on the Floquet-Fourier representation of the solutions of the TDSE describing the helium atom in the presence of the linearly polarized monochromatic electromagnetic field. The resulting set of Floquet equations was solved by means of the CRM method supplemented by the Hylleraas basis technique.

We would like to emphasize the accuracy of the present results for the photoionization cross-sections which is on the level of a fraction of a percent which, we believe, is the most accurate present estimate for the total cross-sections. The interest in obtaining such accurate data in photoionization calculations is two-fold. From the pure theoretical point of view, we tried to demonstrate, that the level of accuracy approaching the standards of the bound state calculations is attainable in the photoionization calculations. On a more practical side, helium is often used as a standard in experiments on photoionization. Achieving such an accuracy in describing the photoionization process in helium provides, therefore, a set of accurate data, which can be used in experiments performed with other gases.

Although only few selected photon energies were reported in the paper, far wider and denser energy grid was covered by the present calculation. These results might serve as an accurate database and find their use in various astrophysics and atomic physics applications. The authors shall gladly communicate these data on request.

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