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High-lying $^{1,3}P^0$ resonance states of He (n = 4) and H^-(n = 5)

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Abstract. The diagonalization approximation is used to investigate the resonance states of He and H^- respectively near the $n = 4$ and $n = 5$ hydrogen thresholds. Computations are carried out for states of $^{1,3}P^0$ symmetries; energies, total and partial widths of autoionization states of helium and autodetaching states of the negative hydrogen ion are calculated. Comparison is made with experiment and theory.

PACS. 32.80.Fb Photoionization of atoms and ions – 32.80.Gc Photodetachment of atomic negative ions

1 Introduction

Studies of autoionization states of helium have received a great deal of attention in recent experiments thanks to the advent of modern synchrotron radiation sources with their associated high-resolution monochromators [1–3]. A set of calculations of the characteristics of double excited resonances in helium have been carried out by various methods using different approaches. Oberoi [4] has calculated the energy position of $(4ln'l')$ doubly excited states of helium with a conventional Feshbach approach by using a hydrogen orbital for the inner electron. The energy calculation of these states has been performed by Herrick and Sinanoglu [5], and Robaux [6] with a modified Feshbach projection formalism such as a truncated diagonalization method in a basis of hydrogen configurations. In addition, Herrick and Sinanoglu [5] have also calculated total widths of the eleven lowest $^1P^0$ and $^3P^0$ resonances. Davis and Chang [7] used the Feshbach saddle point technique to calculate the energies of lowest $^1P^0$ resonances. Ho [8] has used the complex rotation method with Hylleraas basis functions to calculate the resonance positions and total widths of the three lowest $^1P^0$ and $^3P^0$ resonances. Wintgen and Delande [9] have also used the complex rotation method to calculate the resonance positions. Other theoretical calculations of the energies of the $^1P^0$ states are given by Fukuda *et al.* [10] using the diabatic and adiabatic hyperspherical method. Nevertheless, in most of these works only a few calculations have produced a complete set of resonance parameters (resonance position, total and partial widths) for the doubly excited $^{1,3}P^0$ resonances in helium.

Among the two-electron systems, the negative hydrogen ion H^- ($Z = 1$) is also of great interest due to the fact that the electron-electron interaction in H^- is as strong as the nucleus-electron one. These interactions lead to strong correlation effects which explain the existence of shape resonances above threshold in addition to the usual Feshbach resonances which lie below threshold and which are common to any two-electron systems. Such resonances were observed recently [11,12]. These observations are completed by new measurements of field-induced window-type resonances in electron detachment of H^- in the static electric field [13,14]. Few theoretical methods have been used to carry out a complete set of resonance parameters such as energies and widths of $^{1,3}P^0$ states of H^- converging to the $n = 5$ hydrogen threshold. The most intensive calculations in the literature are obtained by using the complex coordinate rotation and have provided the energies and widths of several symmetries up to $n = 9$ threshold [15–17]. There are also some adiabatic calculations using hyperspherical coordinates [18,19]; however, no widths were given in these calculations.

In this work, we have reported calculations of the excitation energies and the total widths of the $^1P^0$ and $^3P^0$ symmetries for several resonances of doubly excited $^{1,3}P^0$ states of He and H^- below the $n = 4$ and 5 hydrogen threshold respectively. In addition we have calculated the partial widths related to the different open channels. These calculations were done in the framework of the diagonalization approximation in the LS coupling scheme. Particular interest of the diagonalization method is to take into account the coupling between closed and open channels in terms of perturbation theory and to neglect the indirect coupling of resonant states through the open channels. This approximation has already been used with success for the description of autoionizing resonances in helium and some helium-like systems converging to $n = 2$, 3 and 4 ionization thresholds of the residual ions [20–26].

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2 Theory

2.1 Basic formulas and approximations

For two-electron systems, the partial amplitude $T_j(E)$ in terms of dipole matrix elements is defined by:

$$T_j(E) = \langle \psi_{Ej} | \widehat{D} | \psi_0 \rangle,$$

where $\widehat{D}$ is the momentum operator, ψ_0 is the atomic initial wave function and ψ_{Ej} is the wave function of the system ion (or hydrogen atom in the case of H^-) + photoelectron in the channel j. In the diagonalization approximation, the final-state wave function is expanded in the subspaces of closed and open channels as follows:

$$\psi_{Ej}(r_1, r_2) = \widehat{A} \sum_k [\psi_k(r_1) U_{kj}(E, r_2)] + \sum_\mu \Lambda_\mu(E) \phi_\mu(r_1, r_2), \quad (1)$$

where $\widehat{A}$ is the operator of antisymetrization, k represents a set of quantum numbers characterizing the final system in the subspace of open channels, and $U_{ki}(E, r_2)$ is an unknown function describing the motion of the photoelectron.

$\psi_k(r_1)$ is the eigenfunction of the residual ion or atom (hydrogen atom in the case of H^-) satisfying the relations:

$$\langle \psi_k | \psi_{k'} \rangle = \delta_{kk'} \quad (2a)$$

$$\langle \psi_k | \hat{H} | \psi_{k'} \rangle = \varepsilon_k \delta_{kk'} + V_{kk'}. \quad (2b)$$

The functions $\phi_\mu(r_1, r_2)$ are obtained by unitary transformation of the Hamiltonian $\widehat{H}$ in the subspace of closed channels:

$$\phi_\mu(r_1, r_2) = \widehat{A} \sum_{lm} \alpha_\mu [\psi_l(r_1) \psi_m(r_2)], \quad (3)$$

with the condition of diagonalization:

$$\langle \phi_\mu | \widehat{H} | \phi_\nu \rangle = E_\mu \delta_{\mu\nu}. \quad (4)$$

The coefficients α_μ of the unitary transformation (3) are found by solving the system of linear algebraic equations:

$$\sum_\nu \left\{ (E_\mu - E_0)\delta_{\mu\nu} - \langle \chi_\mu | \widehat{V} | \chi_\nu \rangle \right\} \alpha_\nu = 0, \quad (5)$$

here $\widehat{V} = 1/|r_1 - r_2|$ (in a.u.) is the electron-electron interaction potential, and E_0 is the energy eigenvalue of the zero-order Hamiltonian $\widehat{H}_0$ corresponding to the eigenfunctions χ_ν defined by:

$$\chi_\mu = \widehat{A}[\psi_l(r_1)\psi_m(r_2)]. \quad (6)$$

The determination of the function $\psi_{Ei}(r_1, r_2)$ is equivalent to the calculation of the coefficients $\Lambda_\mu(E)$ and $U_{ki}(E, r_2)$. Detailed calculations of these coefficients and systems of equations which they satisfy have been reported by Balashov *et al.* [20] and by Wagué [22,26]. From [22], the partial amplitude that describes the formation of a He^+ ion (or a residual neutral hydrogen atom in the case of H^-) and a photoelectron in a definite state has been defined by the following expression:

$$T_j = \langle \varphi_j(E) | \widehat{D} | \psi_0 \rangle + \frac{q+i}{\varepsilon - i} \langle \phi_\mu | \widehat{V} | \varphi_j(E) \rangle \times \frac{\sum_k \langle \phi_\mu | \widehat{V} | \varphi_k(E) \rangle \langle \varphi_k(E) | \widehat{D} | \psi_0 \rangle}{\sum_k |\langle \phi_\mu | \widehat{V} | \varphi_k(E) \rangle|^2}. \quad (7)$$

In (7), $\varphi_j(E)$ is the wave function of the continuous spectrum in the channel j, without resonance interference; $\varepsilon = (E - E_\mu)/(1/2)\Gamma_\mu^{tot}$ is the relative deviation from resonance; E_μ is the energy of the resonant level μ; q is the profile index of the resonance; the sum of integrals in the denominator of (7) determines the total width Γ_μ^{tot} of the autodetaching level μ of H^- (or autoionization states of He). The total width and the profile index are defined respectively by the equations:

$$\Gamma_\mu^{tot} = 2\pi \sum_j |\langle \phi_\mu | \widehat{V} | \varphi_j(E) \rangle|^2 \quad (8a)$$

and

$$q = \frac{\langle \phi_\mu | \widehat{D} | \psi_0 \rangle}{\pi \sum_k \langle \phi_\mu | \widehat{V} | \varphi_k(E) \rangle \langle \varphi_k(E) | \widehat{D} | \psi_0 \rangle}. \quad (8b)$$

2.2 Calculation of the decay probabilities of the resonant states

The autodetachment probabilities of the high-lying states of H^- are obtained by using the approximation involving hydrogen wave functions for the bound electrons with the effective charge $Z = 1$. In this case, the outgoing electron is considered to be free from the residual neutral hydrogen atom, and thus the radial part of the continuum wave functions $\varphi_j(E)$ is described by the normalized spherical Bessel function, to represent a free electron carrying a definite angular momentum l in the channel j. This function has the following form:

$$R_{kl}(r) = \sqrt{\frac{2k}{\pi}} \frac{(2)^l (k)^l l!}{(2l+1)!} r^l e^{ikr} \, {}_1F_1(l+1, 2l+2; 2ikr) \quad (9)$$

where ${}_1F_1(l+1, 2l+2; 2ikr)$ is a confluent hypergeometric function. The spin-angle functions in all cases can be handled by the well-known methods of the Wigner algebra. To determine the autodetachment probability the evaluation

$$R^x(n_1l_1\ n_2l_2 \to n_3l_3\ kl_4) = N_1N_2N_3N_4 \times \sum_{s_1=0}^{n_1-l_1-1} \sum_{s_2=0}^{n_2-l_2-1} \sum_{s_3=0}^{n_3-l_3-1} B(n_1,l_1,s_1)B(n_2,l_2,s_2)B(n_3,l_3,s_3)(\gamma_1+\gamma_3)^{l_1+l_3+s_1+s_2+x+2} \times \Big((l_1+l_3+s_1+s_2+x+2)! \left[J^{l_4}_{l_2+s_2-x}(\gamma_2) - \sum_{t=0}^{l_1+l_3+s_1+s_2+x+2} J^{l_4}_{l_2+s_2-x-t}(\gamma_1+\gamma_2+\gamma_3)\right] + \frac{(l_1+l_3+s_1+s_2-x+1)!}{(\gamma_1+\gamma_3)^{-2x-1}} \sum_{s=0}^{l_1+l_3+s_1+s_2-x+1} J^{l_4}_{l_2+s_2+x+1+s}(\gamma_1+\gamma_2+\gamma_3)\Big) \quad (10)$$

of the following basic type integrals is required [27]:

see equation (10) above

where

$$N_i = \sqrt{\frac{(n_i+l_i)(n_i+l_i-1)}{2n_i}} \left(2\frac{Z_i}{n_i}\right)^{1/2} \quad i = 1,2,3; \quad (11a)$$

$$N_4 = \sqrt{\frac{2k}{\pi}} \frac{(2)^{l_4}(k)^{l_4} l!}{(2l_4+1)!} \quad (11b)$$

$$B_{n_il_is_i} = \frac{(-1)^{s_i}(2\gamma_i)^{l_i+s_i}}{(n_i-l_i-1-s_i)!(2l_i+1+s_i)!s_i!}; \qquad \gamma_i = \frac{Z_i}{n_i} \qquad i = 1,\ 2,\ 3 \quad (12)$$

$$J^l_n(\beta) = \int_0^{+\infty} e^{-(\beta+ik)r_2} r_2^{n+l+1} \times {}_1F_1(l+1, 2l+2, 2ikr_2)dr_2. \quad (13)$$

In the expressions of $J^l_n(\beta)$, ${}_1F_1(a,b,x)$ is a confluent hypergeometric function.

For practical calculations it is convenient to use recurrence relations between these integrals, which can either be obtained by integrating the Schrödinger equation or by using the functional relationships between associated hypergeometric functions ${}_1F_1(a,b;x)$ and ${}_1F_1(a+m,b+n;x)$ and their derivatives [28].

For arbitrary values of n and l the functions $J^l_n(\beta)$ are connected with the functions $J^l_l(\beta)$ and $J^0_{-1}(\beta)$ which can be obtained from the following formulas:

$$J^l_l(\beta) = \frac{(2l+1)!}{(k^2+\beta^2)^{l+1}} \quad (14a)$$

$$J^0_{-1}(\beta) = \frac{1}{k}\arctan\frac{k}{\beta} \quad (14b)$$

$$J^l_{l+1}(\beta) = 2\frac{(l+1)\beta}{k^2+\beta^2} J^0_{-1}(\beta) \quad (14c)$$

$$J^l_{n+2}(\beta) = \frac{2(n+2)\beta J^l_{n+1}(\beta) + [(l+1)-(n+1)(n+2)]J^l_n(\beta)}{k^2+\beta^2} \quad (14d)$$

$$J^l_{n-2}(\beta) = \frac{(k^2+\beta^2)J^l_{n+1}(\beta) + 2n\beta J^l_{n-1}(\beta)}{l(l+1)-n(n+1)} \quad (14e)$$

$$J^l_{l-2}(\beta) = \frac{(2\ell+1)}{k^2}[(2l-1)J^{l-1}_{l-2}(\beta) - \beta J^{l-1}_{l-1}(\beta)] \cdot \quad (14f)$$

For the calculation of the decay probabilities of the resonant states of helium following the works of Brandsen *et al.* [29] and Zemtsov [27] we have used equations similar to equations (10–14) by replacing the Bessel Functions with Coulomb wave functions.

3 Results and discussions

The diagonalization calculations of the excitation energies of the autoionization states of helium are carried out in the 24 × 24 basis which contained configurations: $4ln'l'$ with $n' = 4,\ 5,\ 6,\ 7$. The wave functions are described by the antisymmetric product of the hydrogen wave functions determined in the field of nuclear charge $Z = 2$.

For the excitation energies of the autodetaching states of H^-, we have used the basis of 49 configurations: $nln'l'$ with $n = 5$; $n' \leq 10$ and the hydrogen wave functions used in this case are determined in the field of nuclear charge $Z = 1$. We have converted some resonant parameters in the tables by using the infinite Rydberg constant $R_\infty = 13.605\,698$ eV, and by considering the double-detachment threshold of H^- at 14.3525 eV. In order to compare our results on the helium atom, with those of other theoretical and experimental works, we have adopted the classification scheme of Herrick and Sinanoglu [5]. In this classification new correlation quantum numbers T, K and A were introduced describing the angular (T,K) and radial (A) correlations. In this scheme, the double-excitation states are denoted by $n(K,T)^A_N$ where N and n are respectively inner and outer electrons' quantum numbers. We have labeled our results on helium according to the abbreviated form of the classification scheme of Zubek *et al.* [1] in which the $n(K,T)^A_N$ notation is replaced by N, K_n (in this work $T = 0$ or 1).

Table 1. Energies ($-E$ in a.u.) of the $^1P^0$ autoionizing states of He converging to $N = 4$ threshold of the residual He^+ ion.

	Theoretical results				Experimental results			
States	This work	(a)	(b)	(c)	(d)	(e)	(f)	(g)
2_4	0.1946	0.1946	0.1939	0.1945	0.1930	0.1963	0.1942	0.1943
0_4	0.1760	0.1760	0.1770	0.1788		0.1783	0.1792	0.1791
3_5	0.1688	0.1688	0.1688	0.1688				
1_5	0.1604	0.1604	0.1610					
2_5	0.1603	0.1603	0.1606		0.1605	0.1629	0.1619	0.1610
3_6	0.1517	0.1517	0.1517					
0_5	0.1507	0.1507	0.1510			0.1554	0.1554	0.1511
-1_5	0.1488	0.1488	0.1496					
2_6	0.1473	0.1473	0.1488		0.1474	0.1497	0.1487	0.1478
-2_4	0.1468	0.1468	0.1473					
1_6	0.1465	0.1465	0.1466					

(a) Herrick and Sinanoglu [5]
(b) Brian F Davis and Kwong T Chung [7]
(c) Ho Y.K. [8]
(d) Madden and Codling [30]
(e) Woodruff and Samson [31]
(f) Zubek et al. [1],
(g) Domke et al. [3]

Table 2. Energies ($-E$ in a.u.) of the $^3P^0$ autoionizing states of He converging to $N = 4$ threshold of the residual He^+ ion.

	Theoretical results			
States	This work	(a)	(b)	(c)
3_4	0.2007	0.2007	0.2009	0.2001
1_4	0.1858	0.1858	0.1860	0.1860
2_5	0.1653	0.1653	0.1654	
3_5	0.1645	0.1645	0.1648	
-1_4	0.1613	0.1613	0.1613	
0_5	0.1557	0.1557	0.1557	
1_5	0.1555	0.1553	0.1553	
3_6	0.1497	0.1499	0.1500	
2_6	0.1490	0.1495	0.1494	
-1_5	0.1452	0.1450	0.1450	
1_6	0.1432			

(a) Herrick and Sinanoglu [5]
(b) R.S. Oberoi [4]
(c) Ho Y.K. [8]

Excitation energies of He are reported in Table 1 for $^1P^0$ states and in Table 2 for $^3P^0$ states. A comparison is made with the theoretical results obtained by Ho [8], Herrick and Sinanoglu [5] and Davis and Chung [7], using respectively the complex rotation, the Feshbach truncated diagonalization formalism and the Feshbach saddle point variational technique. Comparison is also made with experimental results of Madden and Codling [30], Woodruff and Samson [31], Zubeket *et al.* [1] and Domke *et al.* [3]. The present calculations are generally in good agreement with existing theoretical data both for $^1P^0$ and $^3P^0$ states, especially with those obtained by Herrick and Sinanoglu [5] using the Feshbach truncated diagonalization formalism which is more complicated than the diagonalization approximation used in our calculations and which in practice entails solving a system of linear algebraic equations.

Concerning the experimental measurements, the data given by Domke *et al.* [3] and Madden and Codling [30] for the $^1P^0$ resonances agree with the present results. In these experimental investigations, only states of the two most intense Rydberg series $(4, 2_n)$ and $(4, 0_n)$, according to the abbreviated form of the $n(K,T)^A_N$ classification scheme [1] were resolved below the $n = 4$ threshold of He^+ and $(4ln'l'')$ triplet resonances of He have not been investigated due to forbidden selection rules in photoionization experiments.

Excitation energies of the negative hydrogen ion are summarized in Table 3 for $^1P^0$ states, in which comparisons are made with other calculations obtained with the complex coordinate rotation [16] and with the adiabatic calculations using hyperspherical coordinates [18,19]; comparisons are also made with experimental measurements [11,14]. Table 4 compares our resonance positions of the $^3P^0$ states with theoretical predictions obtained by using the complex coordinate rotation [15,17]. The present calculations are reasonably in good agreement with existing theoretical and experimental data. However, we have not found a $^1P^0$ resonance at the energy position close to 0.043 629 Ry as obtained by Ho [16] and Koyama *et al.* [18] for the $^1P^0$ states. Concerning the resonance positions of the $^3P^0$ states there are not many published works near the $n = 5$ hydrogen threshold and for these resonances our results are compared with the results given in complex coordinate formalism [17] which concern only the two first resonances. In our knowledge, there is no experimental data for this symmetry.

The total widths of resonance states of He are reported in Table 5 for $^1P^0$ states and Table 6 for $^3P^0$ states. A comparison is made with the theoretical results obtained by Herrick and Sinanoglu [5] and Ho [8] using respectively the Feshbach formalism and the complex rotation method. For $^1P^0$ states, comparison is also made with experimental results obtained by Zubek *et al.* [1] and by Domke *et al.* [3]. Our results agree well with those obtained by Herrick and Sinanoglu [5] both for $^1P^0$ and $^3P^0$ states. For the total widths of the $^3P^0$ (1) and $^3P^0$ (2) states, our results are quite different from Ho's results. Only the width of the $^1P^0$ (2) is close to the one we have calculated. The width of the $^1P^0$ (1) calculated by Ho [8] is about two times the width we have given for the same resonance. One can see that the largest autoionization widths correspond to the resonances of the $(4, 2_n)$, $(4, 0_n)$ and $(4, -2_n)$

Table 3. Energies ($-E$ in Ry) of the $^1P^0$ autodetaching states of the H^- ion converging to $N = 5$ hydrogen threshold.

	Theoretical results				Experimental results	
States	Present	(a)	(b)	(c)	(d)	(e)
5s 5p	0.049159	0.049033	0.04937	0.04900	0.049010	0.048922
5d 5f	0.045202	0.045261	0.04516			
-	-	0.043629	0.04300			
5s 6p	0.042751	0.042656	0.04269	0.04260	0.042762	
5p 8d	0.042486	0.042140	0.04200			
5s 7p	0.042117	0.042063	0.04186			
5f 7g	0.041851	0.040939		0.04090	0.041212	
10s 5p	0.041287	0.040894				
5d 10f	0.040995	0.040486				
10d 5f	0.040393	0.040383				
5d 9f	0.040246					
5p 9d	0.039906					

(a) Ho Y. K. [16]
(b) Koyama et al. [18]
(c) Sadeghpour H. R. [19]
(d) Harris et al. [11]
(e) Halka et al. [14]

Table 4. Energies ($-E$ in Ry) of the $^3P^0$ autodetaching states of the H^- ion converging to $N = 5$ hydrogen threshold.

		Other theoretical results
States	Present	(g)
5s 5p	0.051544	0.0512
5p 5d	0.045967	0.04655
5p 6d	0.043885	
5s 7p	0.043692	
5p 8d	0.041579	
8s 5p	0.041297	
5d 7f	0.041092	
10s 5p	0.040480	
5g 10h	0.040398	
5p 9d	0.040315	
5d 10f	0.040021	
5f 10g	0.039571	0.039902

(g) Ho Y. K. [17].

Table 5. Total widths (Γ_μ^{tot} in eV) of the $^1P^0$ autoionizing states of He converging to $N = 4$ threshold of the residual He^+ ion. The number in parenthesis is the power of ten by which the adjacent number should be multiplied.

States (K_n)	Present work	(a)	(b)	(c)	(d)
2_4	0.464 (-1)	0.46 (-1)	0.98 (-1)	0.89 (-1)	0.94 (-1)
0_4	0.124	0.124	0.129		0.100
3_5	0.223 (-3)	0.226 (-3)	0.1 (-2)		
1_5	0.64 (-2)	0.64 (-2)			
2_5	0.230 (-1)	0.23 (-1)			0.59 (-1)
3_6	0.158 (-3)	0.16 (-3)			
0_5	0.506 (-1)	0.51(-1)			0.66 (-1)
-1_5	0.148 (-2)	0.148 (-2)			
2_6	0.197 (-1)	0.20 (-1)			0.32 (-1)
-2_4	0.266 (-1)				
1_6	0.774 (-3)				

(a) Herrick and Sinanoglu [5]
(b) Ho Y.K. [8]
(c) Zubek et al. [1]
(d) Domke et al. [3]

Table 6. Total widths (Γ_μ^{tot} in eV) of the $^3P^0$ autoionizing states of He converging to $N = 4$ threshold of the residual He^+ ion. The number in parenthesis is the power of ten by which the adjacent number should be multiplied.

States (K_n)	Present work	(a)	(b)
3_4	0.251 (-1)	0.252 (-1)	0.53 (-1)
1_4	0.724 (-1)	0.724 (-1)	0.130
2_5	0.316 (-3)	0.314 (-3)	
3_5	0.206 (-1)	0.206 (-1)	
-1_4	0.553 (-1)	0.574 (-1)	
0_5	0.162 (-2)	0.162 (-2)	
1_5	0.329 (-1)	0.329 (-1)	
3_6	0.125 (-1)	0.126 (-1)	
2_6	0.421 (-3)	0.420 (-3)	
-1_5	0.137 (-1)	0.137 (-1)	
1_6	0.116 (-2)		

(a) Herrick and Sinanoglu [5]
(b) Ho Y.K. [8]

Table 7. Total widths (in Ry) of the $^1P^0$ autodetaching states of the H^- ion converging to $N = 5$ hydrogen threshold. The number in parenthesis is the power of ten by which the adjacent number should be multiplied.

	Theoretical results		Experimental results	
States	Present	(a)	(d)	(e)
Γ (5s 5p)	1.584(-3)	1.536(-3)	1.58 (-3)	1.6(-3)
Γ (5d 5f)	8.3(-5)	4.86(-5)		
-	-	1.013(-3)		
Γ (5s 6p)	1.604(-3)	6.0(-4)	1.036(-3)	
Γ (5p 8d)	3.947(-4)	3.00(-5)		
Γ (5s 7p)	5.234(-5)	3.76(-5)		
Γ (5f 7g)	6.800(-5)	2.4(-4)	1.05(-3)	
Γ (10s 5p)	1.660(-5)	1.4(-5)		
Γ (5d 10f)	2.777(-4)	1.6(-5)		
Γ (10d 5f)	3.505(-5)	1.5(-4)		
Γ (5d 9f)	2.008(-4)			
Γ (5p 9d)	2.19(-4)			

(a) Ho Y. K. [16]
(d) Harris et al. [11]
(e) Halka et al. [14]

Table 8. Total widths (in Ry) of the $^3P^0$ autodetaching states of the H^- ion converging to $N = 5$ hydrogen threshold. The number in parenthesis is the power of ten by which the adjacent number should be multiplied.

	Theoretical calculations	
States	Present	(g)
Γ (5s 5p)	1.566(-3)	1.38(-3)
Γ (5p 5d)	1.983(-3)	1.42(-3)
Γ (5p 6d)	4.519(-4)	
Γ (5s 7p)	7.076(-5)	
Γ (5p 8d)	1.965(-4)	
Γ (8s 5p)	3.287(-5)	
Γ (5d 7f)	2.703(-4)	
Γ (10s 5p)	8.890(-5)	
Γ (5g 10h)	4.713(-4)	
Γ (5p 9d)	4.590(-5)	
Γ (5d 10f)	5.607(-4)	
Γ (5f 10g)	3.356(-5)	2.26(-4)

(g) Ho Y. K. [17]

series for the $^1P^0$ and $(4, 3_n)$, $(4, 1_n)$ and $(4, -1_n)$ for the $^3P^0$. Comparison with the experimental results, show that the widths given by Domke *et al.* [3] for the less broadened secondary series $(4, 0_n)$, agree with our results. In contrast, the widths obtained for the broadened principal series $(4, 2_n)$ are about two times greater than our corresponding results. As mentioned by Domke *et al.* [3], the principal series $(4, 2_n)$ is strongly perturbed by the broadening of resonances. This may explain the large disagreement with our corresponding results. In addition, the computation of the total widths that we have done in different basis, have shown that the values obtained for the $(4, 2_n)$ states are very stable with respect to the dimension of the basis (from 10 to 38), even when including inter-series interaction with high lying-states of the $(5, 3_n)$ series.

The total widths of the negative hydrogen ion, are reported in Table 7 for $^1P^0$ states and Table 8 for $^3P^0$ states. Concerning the $^1P^0$ states, comparison is made with the theoretical results obtained by using the complex coordinate rotation [15–17]. For $^1P^0$ states, comparison is also made with experimental results obtained by Halka *et al.* (1993) and Harris *et al.* (1990). Concerning the $^1P^0$ states, our widths calculations agree well with other results specially for the lowest resonances. For the width of the $^1P^0$ (1) our result is in excellent agreement with experimental measurements.

The partial widths corresponding to decay of the $^{1,3}P^0$ $(n = 4)$ resonances states of He and $^{1,3}P^0$ $(n = 5)$ autodetaching states of H^- through the different open channels are summarized in Tables 9–12. In all case, these partial widths are given in the zero order of direct coupling between different continua and are, and represent the first estimations of the magnitude of the decay of resonances through the related open channels.

Table 9. Partial widths (Γ_j in meV) of the $^1P^0$ autoionizing states of He converging to $N = 4$ threshold of the residual He^+ ion. The number in parenthesis is the power of ten by which the adjacent number should be multiplied.

states	Γ_{1skp}	Γ_{2skp}	Γ_{2pks}	Γ_{2pkd}	Γ_{3skp}	Γ_{3pks}	Γ_{3pkd}	Γ_{3dkp}	Γ_{3dkf}
2_4	0.058	6.911	1.323	1.207	14.496	1.683	18.386	0.460	1.951
0_4	0.089	0.245	0.015	0.003	1.848	2.851	61.457	5.805	52.012
3_5	0.05(-3)	0.009	0.32(-3)	0.003	0.001	0.124	0.036	0.031	0.016
1_5	0.014	1.385	0.226	0.175	2.817	0.643	1.055	0.017	0.072
2_5	0.031	3.493	0.660	0.567	8.289	1.058	7.290	0.242	0.967
3_6	0.04(-3)	0.007	0.63(-3)	0.002	0.02(-2)	0.082	0.029	0.023	0.012
0_5	0.028	0.075	0.028	0.068	1.300	0.702	17.331	2.162	28.931
-1_5	0.34(-3)	0.003	0.12(-3)	0.07(-3)	0.035	0.026	0.157	0.292	0.969
2_6	0.025	3.142	0.641	0.730	7.602	1.314	6.024	0.244	0.013
-2_4	0.018	0.083	0.020	0.957	0.027	0.001	1.264	0.763	23.511
1_6	0.01(-3)	0.007	0.005	0.010	0.058	0.05(-2)	0.377	0.045	0.267

Table 10. Partial widths (Γ_j in meV) of the $^3P^0$ autoionizing states of He converging to $N = 4$ threshold of the residual He^+ ion. The number in parenthesis is the power of ten by which the adjacent number should be multiplied.

states	Γ_{1skp}	Γ_{2skp}	Γ_{2pks}	Γ_{2pkd}	Γ_{3skp}	Γ_{3pks}	Γ_{3pkd}	Γ_{3dkp}	Γ_{3dkf}
3_4	0.123	4.041	1.944	0.762	0.073	0.883	6.604	0.369	0.319
1_4	0.013	1.304	0.020	1.104	1.071	0.003	45.362	7.453	16.068
2_5	0.03(-2)	0.06(-2)	0.002	0.08(3)	0.008	0.066	0.049	0.123	0.064
3_5	0.118	3.585	1.716	0.646	9.009	1.271	3.889	0.226	0.112
-1_4	$< 10^{-5}$	0.066	0.063	0.112	0.810	0.382	11.594	0.840	41.443
0_5	0.002(-2)	0.001	0.003(-1)	0.003	0.044	0.227	0.044	0.127	1.170
1_5	0.009	0.839	0.017	0.553	1.087	0.004	22.310	4.525	3.520
3_6	0.074	2.164	1.057	0.404	5.516	0.843	2.222	0.135	0.113
2_6	0.24(-3)	0.023	0.004	0.003	0.049	0.093	0.113	0.091	0.041
-1_5	0.12(-3)	0.002	0.025	0.011	0.159	0.092	1.521	0.023	11.916
1_6	0.15(-3)	0.031	0.04(-3)	0.036	0.066	0.064	0.386	0.060	0.514

Table 11. Partial widths Γ_j (in meV) of the $^1P^0$ states of the H^- ion converging to $N = 5$ threshold of H, relating to the following open channels j: $1skp$, $2pks$, $2skp$, $2pkd$, $3skp$, $3pks$, $3pkd$, $3dkp$, $3dkf$, $4skp$, $4pks$, $4pkd$, $4dkp$, $4dkf$, $4fkd$, and $4fkg$. The number in parenthesis is the power of ten by which the adjacent number should be multiplied.

states	Γ_{1skp}	Γ_{2skp}	Γ_{2pks}	Γ_{2pkd}	Γ_{3skp}	Γ_{3pks}	Γ_{3pkd}	Γ_{3dkp}	Γ_{3dkf}	Γ_{4skp}	Γ_{4pks}	Γ_{4pkd}	Γ_{4dkp}	Γ_{4dkf}	Γ_{4fkd}	Γ_{4fkg}
5s5p	0.0016	0.0230	0.8481	0.0054	0.2817	0.0001	0.2117	0.9930	0.0228	2.5044	3.1821	1.2808	8.0565	3.8725	0.2728	0.0086
5d5f	< 1(-5)	6 (-5)	2 (-5)	< 1(-5)	4 (-5)	0.0052	0.0026	0.0005	< 1(-5)	0.0003	0.6002	0.4580	0.0002	0.0223	0.0428	0.1572
5s6p	0.0025	0.0851	0.1333	0.2393	0.0054	0.5811	0.6821	3.0969	0.0108	1.0098	0.8839	0.1493	2.7773	8.6746	3.4933	3.7533
5p8d	< 1(-5)	0.0033	0.1770	0.0468	0.1855	0.1260	0.0338	0.1149	0.0006	2.2801	0.3128	0.0069	0.9044	0.3920	0.7862	0.5676
5s7p	< 1(-5)	1(-5)	8(-5)	< 1(-5)	< 1(-5)	0.0023	0.0011	0.0003	< 1(-5)	0.0328	0.2442	0.3150	0.0312	0.0474	0.0377	0.0242
5f7g	1(-5)	1.3(-4)	1.5(-4)	0.0010	0.0017	0.0012	0.0047	0.0164	1.4(-4)	0.1019	0.0668	0.0660	0.0125	0.3259	0.3266	0.0138
10s5p	1(-5)	0.0003	0.0047	0.0004	0.0006	0.0050	1.7(-4)	0.0093	0.0006	0.0326	0.0737	0.0217	0.0398	0.0338	0.0034	0.0558
5d10f	0.0011	0.0020	0.1855	0.0421	0.0219	0.0438	0.2059	0.3676	0.0809	0.0383	0.0132	0.0301	2.3661	0.2967	0.0827	1.3(-4)
10d5f	1(-5)	0.0003	0.0011	0.0008	1.4(-4)	0.0005	0.0062	0.0016	5(-5)	0.0611	0.0673	0.0022	0.0168	0.1541	0.1645	0.0014
5d9f	1(-5)	0.0399	0.0436	0.1171	0.3675	0.1061	0.7434	0.0008	0.0658	0.4877	0.0656	0.2409	0.0006	0.0529	0.3996	0.1571
5p9d	0.0003	1.2(-4)	0.0074	0.0003	0.2270	0.0032	0.0617	0.3063	0.0311	1.0125	0.6331	0.0069	0.0659	0.3830	0.2403	0.3618
7f5g	1.3(-4)	0.0008	0.0056	0.0049	0.0001	0.0152	0.0195	0.1409	7 (-5)	0.0460	0.0161	0.0994	0.0093	0.6103	0.5339	0.0115
5d8f	5(-5)	0.0018	0.0271	0.0038	0.0187	0.0171	0.0317	0.0974	2(-5)	0.2379	0.0784	1(-5)	0.1023	0.2221	0.1443	0.0538

Table 12. Partial widths Γ_j (in meV) of the $^3P^0$ states of the H^- ion converging to $N = 5$ threshold of H, relating to the following open channels j: $1skp$, $2pks$, $2skp$, $2pkd$, $3skp$, $3pks$, $3pkd$, $3dkp$, $3dkf$, $4skp$, $4pks$, $4pkd$, $4dkp$, $4dkf$, $4fkd$, and $4fkg$. The number in parenthesis is the power of ten by which the adjacent number should be multiplied.

states	Γ_{1skp}	Γ_{2skp}	Γ_{2pks}	Γ_{2pkd}	Γ_{3skp}	Γ_{3pks}	Γ_{3pkd}	Γ_{3dkp}	Γ_{3dkf}	Γ_{4skp}	Γ_{4pks}	Γ_{4pkd}	Γ_{4dkp}	Γ_{4dkf}	Γ_{4fkd}	Γ_{4fkg}
5s5p	0.0139	0.0065	0.2996	0.0204	0.5576	0.0948	0.0797	0.2147	0.0100	4.1820	9.5428	3.2017	1.7238	1.0896	0.2791	0.4374
5p5d	0.0030	0.0260	0.0801	0.0057	0.1632	0.0009	0.2181	1.5547	0.1785	3.7567	0.0284	0.0222	9.7790	11.054	0.1128	0.8412
5p6d	0.0085	0.0056	0.1511	0.0086	0.3380	0.0117	0.0225	0.0687	0.0012	3.9385	0.1102	0.0006	1.2559	0.2247	0.0032	1.8(-4)
5s7p	<1 (-5)	1.7(-4)	<1 (-5)	<1 (-5)	1.8(-4)	0.0033	0.0041	0.0020	<1 (-5)	0.0002	0.2666	0.3933	0.0095	0.1210	0.1624	3.6(-4)
5p8d	0.0042	0.0015	0.1009	0.0098	0.1282	0.0093	0.0074	0.0707	0.0024	1.2901	1.5(-4)	0.0155	0.8564	0.1780	2 (-5)	0.0061
8s5p	1 (-5)	1 (-5)	6.6(-4)	2 (-5)	8.7(-4)	1.6(-4)	0.0021	0.0019	9(-5)	0.0331	0.0883	0.1108	0.0190	0.1164	0.0737	0.0049
5d7f	5.5(-4)	0.0036	0.0078	7(-5)	0.0158	0.0036	0.0483	0.2569	0.0244	0.4589	0.0242	0.1838	1.0487	1.2245	0.3765	0.3551
10s5p	0.0017	0.0064	0.0031	0.0029	0.1313	0.0001	0.0015	0.0229	0.0019	0.6327	0.0130	0.2181	0.0124	0.1054	0.0560	2.6(-4)
5g10h	0.0021	0.0088	7.7(-4)	0.0201	0.2315	0.0431	0.0386	0.0972	0.0126	1.0702	0.1519	0.0222	0.2259	0.3561	0.0500	0.0155
5p9d	8.3(-4)	0.0025	2.4(-4)	0.0106	0.0944	0.0157	0.0278	0.0247	0.0143	0.2553	0.0271	0.0038	0.0969	0.0057	0.0446	0.0854
5d10f	0.0043	0.0017	0.1503	0.0078	0.2115	7.9(-4)	0.0458	0.3403	0.0190	2.6239	0.0496	0.2516	2.7622	1.0034	0.1565	0.0522
5f10g	1(-5)	6(-5)	8.2(-4)	7.5(-4)	0.0018	0.0039	4.7(-4)	8(-5)	<1(-5)	0.0642	0.0758	0.0498	0.0654	0.1480	0.0454	0.0212
7s5p	6(-5)	5.1(-4)	0.0105	0.0246	0.0126	0.0699	0.0702	0.0476	0.0066	0.0073	0.0047	0.0853	0.1113	0.3918	1.1017	0.8400

4 Conclusion

The resonance parameters of He such as excitation energies and total widths reported here are in good agreement with other theoretical calculations except the results obtained by Ho in the complex rotation method. Concerning the $(4, 2_n)$ broadened series of He it should be important to have new experimental data on the total width of these resonances for better understanding of theoretical results. Concerning the $^{1,3}P^0$ $(N = 5)$ resonance parameters of H^-, the results reported here are in good agreement with other theoretical calculations and experimental data. In the calculation of the total widths, a simple treatment of the continuum has provided widths in good agreement with experimental measurements and theoretical calculations reported here, especially for the H^- ion. Nevertheless for better understanding of intra-channel process in the decay of doubly-excited in two-electron systems it will be of interest to look at the higher order approximation in the determination of the partial widths.

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