# Photoejection with excitation in H<sup>-</sup> and other systems

## A. K. Bhatia and R. J. Drachman

Heliophysics Science Division, NASA/Goddard Space Flight Center, Greenbelt, Maryland 20771, USA (Received 5 September 2014; revised manuscript received 19 September 2014; published 5 January 2015)

Lyman- $\alpha$  radiation, 1216 Å, has been seen from the sun and from various astrophysical sources. This radiation arises from the radiative transition from the 2p  $^2P$  state to the 1s  $^2S$  state of the hydrogen atom. The  $^2P$  state can be excited from the 1s  $^2S$  state by electron impact. However, it is possible to produce this excited state by photodetachment of the H<sup>-</sup> ion, leaving the H atom in the  $^2P$  state. We have calculated cross sections for this process using Hylleraas-type functions for the H<sup>-</sup> ion and using the exchange approximation for the photoelectron in the final continuum states of angular momenta equal to 0 and 2. The photoabsorption cross sections in H<sup>-</sup> ions or He atoms leaving the hydrogen atom and helium ion in 2  $^2S$  are also calculated. Similar calculations have been carried out for the Li<sup>+</sup>, Be<sup>2+</sup>, and C<sup>4+</sup> ions.

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### I. INTRODUCTION

Since hydrogen is the most abundant element in the universe it is important and useful to understand all the processes that can contribute to the production of hydrogen spectral lines, especially Lyman  $\alpha$ , the radiation due to the transition between quantum levels n=2 and 1. Recently this radiation has been detected [1] from the Milky Way galaxy, increasing astrophysical interest. The most direct process exciting the n=2 level of hydrogen is electron impact on the ground-state atom. Also important is the similar process of direct photoexcitation. A second-order process in which one photon ionizes one of the electrons and a second photon excites the second electron to the n=2 level also occurs.

Another interesting process resulting in Lyman- $\alpha$  radiation is the single photodetachment of the hydrogen negative ion with excitation of the second electron to the n = 2P level of the remaining hydrogen atom. This process involves the so-called "shake-up" of the second electron, and it is this process that we examine in the present work. Although this is quite simple to formulate it seems not to have been considered much in the past. Perhaps the relative scarcity of the negative ion in astrophysical sources is responsible for this apparent lack of interest, but we think the process is important from the point of view of completeness, and in this paper we treat it carefully. Other systems (helium atoms and the two-electron ions of lithium, beryllium, and carbon) also may give rise to analogous Lyman- $\alpha$  radiation, and can be treated in the same way. In addition, excitation to the 2S state does not yield Lyman- $\alpha$ photons directly, but instead gives two photons sharing the available energy.

In fact, the list of previous ionization-excitation calculations is quite short. A good introduction to the shake-up theory is by Åberg [2]. Jacobs [3] as well as Bell  $et\ al.$  [4] have calculated low-energy photoionization with excitation from the ground state of helium. Drukarev  $et\ al.$  [5] have calculated the process of interest but only for atomic helium and positive heliumlike ions, with the final-state Coulomb wave function to lowest order and for intermediate energies. Forrey  $et\ al.$  [6] have calculated in photoionization of helium atoms at high photon energies the ratios of leaving the remaining electron in the (ns) state to that leaving it in the (1s) state. Their calculation was carried out to infer photoionization to (1s) state also. Kheifets

and Bray [7] have employed the converged close-coupling formalism at high photon energies to calculate photoionization with excitation and double-photoionization cross sections of helium isoelectronic systems. Nefiodov [8] has considered ionization and excitation in high-energy photon scattering. Finally, Kleiman *et al.* [9] treat only the two-electron lithium ion. We are mostly interested here in the ionization-excitation of H<sup>-</sup>, but we also include results for a suite of other two-electron atoms and ions.

The method used is fairly straightforward. It is first order in the dipole operator representing the incident photon, and the initial target is in the form of a Hylleraas-correlated function. The final state is a symmetrized product of the appropriate single-electron ion or atom and the scattering function of the ejected electron in the exchange approximation. Since the observation of Lyman- $\alpha$  radiation is of principal interest, as mentioned above, we emphasize the  $^2P$  final state, but results for the  $^2S$  state are also given.

### II. CALCULATIONS

The photoionization process is given by

$$hv + \text{He} \rightarrow \text{He}^+ + e,$$
 (1)

where He<sup>+</sup> is in the  $^2P$  or  $^2S$  state. The outgoing photoelectron is in the angular momentum  $l_f=0$  or 2 when the resulting state is  $^2P$  and  $l_f=1$  when the resulting state is  $^2S$ . Similar processes take place when the target is H<sup>-</sup>. The cross section for this process in the dipole approximation is given by

$$=\frac{4\pi\alpha k\omega}{3(2l_i+1)}(|M_0|^2+|M_2|^2),\tag{2}$$

for  ${}^{2}P$  states and

$$=\frac{4\pi\alpha k\omega}{3(2l_i+1)}|M_1|^2,\tag{3}$$

for <sup>2</sup>S states. The matrix M is defined as

$$M_{l_f} = (2l_f + 1)^{\frac{1}{2}} |\langle \psi_f | z_1 + z_2 | \phi_i \rangle|.$$
 (4)

In Eq. (3),  $\alpha$  is the fine-structure constant,  $\phi_i$  is the initial bound-state *S*-state wave function of Hylleraas type for H<sup>-</sup> or He with  $l_i=0$ . The number of terms in the bound-state

function is 364 for H<sup>-</sup> and 220 for He and is given by

$$\phi_i(r_1, r_2, r_{12}) = \sum_{lmn}^{N} C_{lmn} \left[ \exp(-ar_1 - br_2) r_1^{l} r_2^{m} r_{12}^{n} + (1 \leftrightarrow 2) \right].$$
 (5)

The C's are the eigenvectors and a and b are the nonlinear parameters.  $\Psi_f$  is the final continuum wave function of the outgoing photoelectron with momentum k, angular momentum  $l_f$ , and  $\omega$  is the energy of the incident photon:

$$\omega = I + k^2. \tag{6}$$

I is the ionization potential of the system absorbing the incident photon and  $k^2$  is the energy of the outgoing photoelectron, and they are in Rydberg units. Since  $k^2$  is in the continuum, absorption is possible for a continuous range of  $\omega$ . Therefore for  $^2P$  states, the total cross section is obtained by using the sum of the cross sections:

$$6 = 6(l_f = 0) + 6(l_f = 2).$$
 (7)

Here we use the length form of the cross section. As stated earlier, parity conservation does not allow  $l_f$  equal to 1 for  $^2P$  states. The final-state wave function is given by

$$\psi_L(\mathbf{r}_1, \mathbf{r}_2) = \mathbf{u}(\mathbf{r}_1) \boldsymbol{\phi}_2(\mathbf{r}_2) \pm (\mathbf{1} \leftrightarrow \mathbf{2}), \tag{8}$$

where  $\phi_2$  is the 2p wave function of the ion or atom with angular momentum equal to 1 for  $^2P$  states and is the 2s wave function for  $^2S$  states, and  $u(r_1)$  is the continuum function. The upper sign in the above equation refers to the singlet states, and the lower sign to the triplet states. The unperturbed radial parts of the target wave functions are given by

$$\phi_{2p}(r_2) = \left(\frac{Z^5}{24}\right)^{1/2} r_2 \exp(-zr_2/2),$$
 (9)

$$\phi_{2s}(r_2) = (Z^3/8)^{1/2}(2 - Zr_2)\exp\left(-\frac{Zr_2}{2}\right).$$
 (10)

TABLE I. Phase shifts (radians) for scattering of electrons (L=0 and 2) from the 2  $^2P$  state in H atoms and He ions in the exchange approximation.

	Electron-H		Electron-He <sup>+</sup>		Electron-Li <sup>+</sup>	
K	L = 0	L=2	L=0	L=2	L=0	L=2
0.1	2.6236		2.4167	1.4789	2.6394	
0.2	2.2242	3.0029	2.3283	1.6580	2.1104	-1.6060
0.3	2.0413	2.8819	2.2473	1.8135	2.0624	-1.5073
0.4	2.0724	2.7746	2.1721	1.9471	2.0154	-1.4117
0.5	2.1422	2.7386	2.1014	2.0644	1.9696	-1.3197
0.6	2.1375	2.7985	2.0338	2.1717	1.9247	-1.2321
0.7	2.0779	2.9373	1.9687	2.2732	1.8807	-1.1484
0.8	1.9964	2.7540	1.9057	2.3712	1.8378	-1.0687
0.9	1.9103	3.2482	1.8451	2.4655	1.7960	-9.9319(-1)
1.0	1.8262	3.3574	1.7865	2.5549	1.7553	-9.2164(-1)
1.1			1.7301	2.6379	1.7154	-8.5409(-1)
1.2			1.6761	2.7133	1.6765	-7.9058(-1)
1.3			1.6244	2.7807	1.6387	-7.3110(-1)
1.4			1.5750	2.8402	1.6018	-6.7566(-1)
1.5			1.5279	2.8922	1.5660	-6.2412(-1)
1.6			1.4830	2.9375	1.5311	-5.7636(-1)
1.7			1.4404	2.9769	1.4972	-5.4228(-1)

TABLE II. Convergence of the photon absorption cross section with respect to the number of terms in the bound-state wave function.

H-	N = 220	N = 286	N = 364
	1.6570	1.6604	1.6578
Не	N = 120	N = 165	N = 220
	3.0458(-2)	3.0395(-2)	3.0459(-2)

The scattering equation for the function  $u(r_1)$  is obtained from the ansatz,

$$\int Y_{L0}(\Omega_1)\phi(r_2)(H-E)\psi_f d\mathbf{r}_2 d\Omega_1 = 0, \qquad (11)$$

where H is the Hamiltonian and E is the total energy of the electron-target system. We have in Rydberg units,

$$H = -\nabla_1^2 - \nabla_2^2 - \frac{2Z}{r_1} - \frac{2Z}{r_2} + \frac{2}{r_{12}},\tag{12}$$

and

$$E = k^2 - Z^2/4, (13)$$

where  $k^2$  is the kinetic energy of the outgoing photoelectron, and Z is the nuclear charge, which is 1 for  $H^-$  and 2 for He. The integrodifferential equation for the scattering function  $u(r_1)$  is obtained from Eq. (11). The phase shifts are obtained from  $u(r_1)$  for  $r_1$  approaching infinity. In Table I, we give the phase shifts for L=0 and 2.

Table II indicates the convergence of the cross section when the final state is  ${}^{2}P$  with respect to the number of terms in the bound-state function for k = 0.30. In Table III, we give the photoabsorption cross sections for H<sup>-</sup> and He for various

TABLE III. Total photoabsorption cross sections (Mb) for the  $^{1}S$  states of the H ion, He, Li<sup>+</sup>, Be<sup>2+</sup>, and C<sup>4+</sup>. The final state is the 2  $^{2}P$  state

K	H-	Не	Li <sup>+</sup>	Be <sup>2+</sup>	C <sup>4+</sup>
0.1	1.2511	3.4706(-2)			
0.2	1.6983	3.2972(-2)	3.8740(-3)	6.9296(-3)	1.8170(-4)
0.3	1.6578	3.0459(-2)	3.8183(-3)	6.7374(-3)	1.8144(-4)
0.4	1.1709	2.7627(-2)	3.7482(-3)	6.4820(-3)	1.8104(-4)
0.5	6.4369(-1)	2.4948(-2)	3.6694(-3)	6.1657(-3)	1.8048(-4)
0.6	4.4867(-1)	2.2717(-2)	3.5894(-3)	5.8193(-3)	1.7987(-4)
0.7	4.1448(-1)	2.1120(-2)	3.5102(-3)	5.4450(-3)	1.7916(-4)
0.8	3.5327(-1)	2.0058(-2)	3.4337(-3)	5.0471(-3)	1.7836(-4)
0.9	2.6847(-1)	1.9375(-2)	3.3712(-3)	4.6498(-3)	1.7505(-4)
1.0	1.508(-1)	1.8811(-2)	3.3083(-3)	4.2507(-3)	1.7641(-4)
1.1		1.8219(-2)	3.2481(-3)	3.8543(-3)	1.7552(-4)
1.2		1.7409(-2)	3.1894(-3)	3.4825(-3)	1.7437(-4)
1.3		1.6392(-2)	3.1220(-3)	3.1270(-3)	1.7322(-4)
1.4		1.5181(-2)	3.0533(-3)	2.8077(-3)	1.7198(-4)
1.5		1.3866(-2)	2.9777(-3)	2.4963(-3)	1.7072(-4)
1.6		1.2498(-2)	2.8919(-3)	2.2171(-3)	1.6963(-4)
1.7		1.1158(-2)	2.7898(-3)	1.9516(-3)	1.6819(-4)
1.8		9.8391(-3)	2.6849(-3)	1.7123(-3)	1.6678(-4)
1.9		8.6095(-3)	2.5735(-3)	1.4960(-3)	1.6521(-4)
2.0		7.4791(-3)	2.4546(-3)	1.3015(-3)	1.6371(-4)

TABLE IV. Phase shifts (radians) for scattering of electrons (L=1) from 2  $^2S$  state in H atoms and He and Li<sup>+</sup> ions in the exchange approximation.

K	Electron-H	Electron-He <sup>+</sup>	Electron-Li <sup>+</sup>
0.1	-8.5249(-2)	-6.2699(-1)	
0.2	-3.7221(-1)	-5.8601(-1)	-2.1108(-1)
0.3	-6.5711(-1)	-5.2364(-1)	-2.0383(-1)
0.4	-7.8181(-1)	-4.4943(-1)	-1.9476(-1)
0.5	-6.7937(-1)	-3.7496(-1)	-1.8475(-1)
0.6	-4.5940(-1)	-3.0968(-1)	-1.7460(-1)
0.7	-3.0539(-1)	-2.5810(-1)	-1.6491(-1)
0.8	-2.3902(-1)	-2.2039(-1)	-1.5605(-1)
0.9	-2.1910(-1)	-1.9445(-1)	-1.4817(-1)
1.0	-2.1890(-1)	-1.7743(-1)	-1.4158(-1)
1.1		-1.6673(-1)	-1.3613(-1)
1.2		-1.6038(-1)	-1.3174(-1)
1.3		-1.5691(-1)	-1.2827(-1)
1.4		-1.5531(-1)	-1.2559(-1)
1.5		-1.5482(-1)	-1.2357(-1)
1.6		-1.5497(-1)	-1.2203(-1)
1.7		-1.5566(-1)	-1.2075(-1)
1.8		-1.5659(-1)	-1.1963(-1)
1.9		-1.5763(-1)	-1.1900(-1)
2.0		-1.5871(-1)	-1.1857(-1)

momenta of the outgoing electron, the number of terms being 364 for H<sup>-</sup> and 220 for He. Since the 2p  $^2P$  state lies above the ground state of the atom or ion, much higher photon energy is required for photon absorption. It is seen from the table that there is a maximum in the photoabsorption cross sections at k = 0.20 for H<sup>-</sup> ion while the cross section decreases monotonically with respect to k in the case of He atom. These cross sections are small compared to the direct excitation of  $^2P$  and  $^2S$  states from the 1s  $^2S$  state by electron impact; nevertheless the photoabsorption process must be considered in the formation of these states. Cross sections for photoabsorption in Li<sup>+</sup>, Be<sup>2+</sup>, and C<sup>4+</sup> are also given in Table III. It is seen that the cross sections decrease as Z is increased up to 3, increase for Z = 5, and decrease again for Z = 6.

A similar calculation has been carried out when the final state is a  ${}^2S$  state. The phase shifts, in the exchange approximation, are given in Table IV.

Table V indicates the convergence of the cross section with respect to the number of terms in the bound-state function for k = 0.3, when the final state is  ${}^2S$ . Cross sections for various k values of the photoelectron are given in Table VI. In the case of the H<sup>-</sup> ion, they are seen to go to zero as  $k \to 0$  and they increase as k increases, with a maximum at k = 0.7, while

TABLE V. Convergence of the photon absorption cross section with respect to the number of terms in the bound-state wave function. The final state is  ${}^2S$ .

H-	N = 220	N = 286	N = 364
Не	7.9246(-2) $N = 120$	7.9145(-2) $N = 165$	8.0269(-2) N = 220
	6.5632(-2)	6.5634(-2)	6.5632(-2)

TABLE VI. Total photoabsorption cross sections (Mb) for the  $^1S$  state of the H ion, He, Li $^+$ , Be $^{2+}$ , and C $^{4+}$  ions. The final state is the  $^2S$  state.

K	H-	Не	Li <sup>+</sup>	Be <sup>2+</sup>	C <sup>4+</sup>
0.1	1.7714(-3)	5.8202(-2)			
0.2	1.5397(-2)	6.1430(-2)	1.2677(-2)	5.9255(-1)	6.0855(-4)
0.3	8.0269(-2)	6.5632(-2)	1.2572(-2)	5.8736(-1)	6.0784(-4)
0.4	3.4131(-1)	6.9367(-2)	1.2431(-2)	5.8031(-1)	6.0692(-4)
0.5	1.0449	7.1535(-2)	1.2259(-2)	5.7132(-1)	6.0544(-4)
0.6	1.7984	7.1897(-2)	1.2067(-2)	5.6085(-1)	6.0363(-4)
0.7	1.9968	7.0903(-2)	1.1864(-2)	5.4890(-1)	6.0209(-4)
0.8	1.8926	6.9150(-2)	1.1650(-2)	5.3579(-1)	6.0014(-4)
0.9	1.7128	6.7067(-2)	1.1430(-2)	5.2136(-1)	5.9798(-4)
1.0	1.5202	6.4859(-2)	1.1210(-2)	5.0609(-1)	5.9486(-4)
1.1		6.2589(-2)	1.0989(-2)	4.9019(-1)	5.9191(-4)
1.2		6.0250(-2)	1.0766(-2)	4.7378(-1)	5.8884(-4)
1.3		5.7839(-2)	1.0541(-2)	4.5704(-1)	5.8556(-4)
1.4		5.5290(-2)	1.0310(-2)	4.4409(-1)	5.8207(-4)
1.5		5.2653(-2)	1.0073(-2)	4.2307(-1)	5.7833(-4)
1.6		4.9922(-2)	9.8295(-3)	4.0603(-1)	5.7456(-4)
1.7		4.7121(-2)	9.5753(-3)	3.8913(-1)	5.7060(-4)
1.8		4.4281(-2)	9.3103(-3)	3.7214(-1)	5.6653(-4)
1.9		4.1433(-2)	9.0380(-3)	3.7214(-1)	5.6219(-4)
2.0		3.8608(-2)	8.7561(-3)	3.3885(-1)	5.5698(-4)

in the case of the He atom, the cross sections are finite as  $k \to 0$ . The behavior of the cross sections is exactly the same as in the photoabsorption when the final state is the  $1s^2S$  state [10]. These cross sections decrease up to Z=3 and then start increasing.

We find in He the ratio of the cross section for the electron in the n = 2 <sup>2</sup>S state to the cross section for the electron in n = 1 after photoionization equal to 0.0535 at  $k^2 = 4$  Ry while in [7] it is 0.0446 in the asymptotic region, a reasonable agreement.

Figure 1 shows cross sections for the H<sup>-</sup> ion. The lower curve is obtained when the final state is the n = 2 <sup>2</sup>S state and

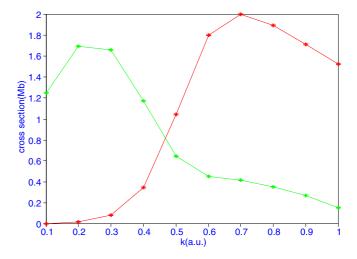


FIG. 1. (Color online) Photodetachment cross section of a hydrogen negative ion. The lower curve (starting from left) is for the excitation to n=2  $^2S$  state and the upper curve is for the excitation to n=2  $^2P$  state.

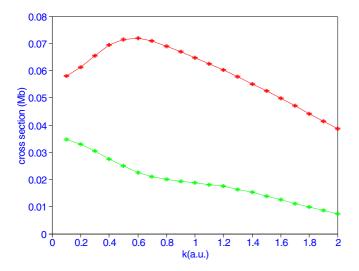


FIG. 2. (Color online) Photoionization cross sections of He. Here the lower curve is for the excitation to n = 2 <sup>2</sup>P state and the upper curve is for excitation to n = 2 <sup>2</sup>S state.

the upper curve is for the n = 2  $^2P$  state. There is a maximum in the cross sections for the  $^2S$  state as well as in the  $^2P$  state. Figure 2 shows cross sections for He and it is seen that the cross sections have a maximum value for the  $^2S$  state and are higher than those for the  $^2P$  state, which decrease with k.

Similar calculations have been carried out for the  $\mathrm{Li}^+, \mathrm{Be}^{2+},$  and  $\mathrm{C}^{4+}$  ions. The number of Hylleraas-type functions are 165 for  $\mathrm{Li}^+,$  and  $\mathrm{Be}^{2+}$  and 120 for the  $\mathrm{C}^{4+}$  ions, respectively. These cross sections are given in Table VI. These results should be useful to infer cross sections for  $\mathrm{B}^{3+}$  by interpolation.

We find in the photoabsorption of the  $H^-$  ion that the cross sections for excitation to the 2  $^2P$  state are larger than those for the 2  $^2S$  state at low photon energies, while the situation is reversed at high photon energies. However, in other systems studied here, cross sections for excitation to the 2  $^2S$  state are always higher than those for the 2  $^2P$  state.

Table VII gives the ratio of cross sections for leaving the target H<sup>-</sup> ions, He atoms, and Li<sup>+</sup> ions in the excited n=2  $^2S$  state and ( $^2S$  and  $^2P$ ) states to the n=1  $^2S$  state after photoabsorption [10]. It should be possible to measure this ratio experimentally. For He atom, Fig. 3 shows the ratios ( $R_1$ ) of the cross sections for 2  $^2S$  to the cross section for the remaining electron in the 1  $^2S$  state. This figure also shows the ratio ( $R_2$ ) when both n=2 excited states are included. We find, compared to all the systems, that  $R_2$  is maximum for H<sup>-</sup>, in agreement with the conclusion in Ref. [7].

# III. RADIATIVE ATTACHMENT

The radiative attachment plays an important role in the solar and astrophysical problems.

$$e + H \rightarrow H^- + h\nu.$$
 (14)

The hydrogen atom is in the  ${}^2S$  or  ${}^2P$  state and the H<sup>-</sup> ion is in the  $(1s^2){}^1S$  state after attachment. H atom in (14) can be replaced by other positively charged ions. This process is an exothermal process and has a small radiative-attachment cross section compared to the photoabsorption cross section  $\sigma$ . The

TABLE VII. Ratios  $R_1$  and  $R_2$  in H<sup>-</sup>, helium atom, and Li<sup>+</sup> ion.

	ion	
k	$R_1^a$	$R_2^{a}$
0.1	1.1760(-4)	8.1873(-2)
0.2	3.9946(-4)	4.4460(-2)
0.3	2.2783(-3)	4.9332(-2)
0.4	1.3944(-2)	6.1779(-2)
0.5	6.4958(-2)	1.0498(-1)
0.6	1.6743(-1)	2.0920(-1)
0.7	2.6673(-1)	3.2210(-1)
0.8	3.3490(-1)	3.9742(-1)
	He atom	
0.1	8.0146(-3)	1.2794(-2)
0.2	8.6667(-3)	1.3318(-2)
0.3	9.6384(-3)	1.4112(-1)
0.4	1.0774(-2)	1.5065(-1)
0.5	1.1935(-2)	1.6097(-2)
0.6	1.3075(-2)	1.7206(-2)
0.7	1.4252(-2)	1.8497(-2)
0.8	1.5551(-2)	2.0062(-2)
0.9	1.7067(-2)	2.1998(-2)
1.0	1.8839(-2)	2.4303(-2)
1.1	2.0919(-2)	2.7008(-2)
1.2	2.3322(-2)	3.0061(-2)
1.3	2.6064(-2)	3.3451(-2)
1.4	2.9114(-2)	3.7107(-2)
1.5	3.2502(-2)	4.1061(-2)
1.6	3.6220(-2)	4.5288(-2)
1.7	4.0175(-2)	4.9688(-2)
1.8	4.4590(-2)	5.4337(-2)
1.9	4.9040(-2)	5.9187(-2)
2.0	5.3511(-2)	6.3877(-2)
	Li <sup>+</sup> ion	
0.2	4.9346(-3)	6.4426(-3)
0.3	4.9889(-3)	6.5041(-3)
0.4	5.0594(-3)	6.5849(-3)
0.5	5.1422(-3)	6.6814(-2)
0.6	4.0317(-3)	5.2310(-3)
0.7	5.3781(-3)	6.9693(-3)
0.8	5.5344(-3)	7.1657(-3)
0.9	5.7203(-3)	7.4081(-3)
1.0	5.9438(-3)	7.6979(-3)
1.1	6.2085(-3)	8.0436(-3)
1.2	6.5170(-3)	8.4476(-3)
1.3	6.8761(-3)	8.9126(-3)
1.4	7.2914(-3)	9.4507(-3)
1.5	7.7664(-3)	1.0062(-2)
1.6	8.3090(-3)	1.0753(-2)

 $\overline{R_1 = \sigma(2^2S)/\sigma(1^2S)}$  and  $R_2 = [\sigma(2^2S) + \sigma(2^2P)]/\sigma(1^2S)$ .

attachment cross section  $\sigma_a$  is given by

$$\sigma_a = \left(\frac{h\upsilon}{cp_e}\right)^2 \frac{g(f)}{g(i)}\sigma = \left(\frac{h\upsilon}{c}\right)^2 \frac{1}{2mE} \frac{g(f)}{g(i)}\sigma. \tag{15}$$

The above expression follows from the principle of detailed balance. In the above equation  $p_e \equiv k$  is the electron momentum, and g(i) and g(f) are the statistical weight factors for the initial and final states. The radiative rate coefficient averaged

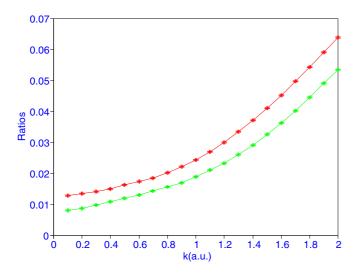


FIG. 3. (Color online) The lower curve is the ratio of cross sections in He for excitation to  $2^2S$  to cross sections for electron to be in the  $1^2S$  state after photoabsorption, and the upper curve represents the ratio of cross sections for excitation to n=2 states to cross sections for electron to be in the  $1^2S$  state after photoabsorption.

over the Maxwellian velocity distribution f(E) is given by

$$\alpha_R(T) = \langle \sigma_a v_e f(E) \rangle.$$
 (16)

The electron velocity is  $v_e$ , and the rate is given by

$$\alpha_R(T) = \left(\frac{2}{\pi}\right)^{1/2} \frac{c \, g(f)}{\left(mc^2 k_B T\right)^{3/2}} \int_0^\infty dE (E+I)^2 \Sigma(E) e^{-\frac{E}{k_B T}}.$$
(17)

TABLE IX. Ground-state energies of two-electron systems.

System	N	a, b	Energy (Ry)
H-	364	1.27, 0.58	-1.0550 1968
Не	220	3.22, 2.17	-5.80744872
Li <sup>+</sup>	165	4.32, 3.40	-14.55982670
$Be^{2+}$	165	2.32, 5.11	-18.36974677
$C^{4+}$	120	9.90, 6.40	-64.81249274

where

$$\Sigma(E) = \left[\frac{\sigma(E)}{g(i)}\right]_{l_i=0} + \left[\frac{\sigma(E)}{g(i)}\right]_{l_i=2}, \text{ for } {}^2P \text{ states.}$$
 (18)

$$\Sigma(E) = \left[\frac{\sigma(E)}{g(i)}\right]_{l_i = 1}, \quad \text{for } {}^2S \text{ states.}$$
 (19)

The photoabsorption cross sections in Eqs. (18) and (19) are in units of  $10^{-18}$  cm<sup>2</sup>. The rate coefficients from the final states 2  $^2P$  and 2  $^2S$  of H and He<sup>+</sup> are given in Table VIII. Most of the contribution to the integral is from the first few energy points. The rate coefficients increase as the electron temperature increases in the case of the H and decreases in the case of the He<sup>+</sup> ion.

Table IX gives the ground-state energies of the  $1s^2$   $^1S$  state, the nonlinear parameters a and b, and the number of terms in Eq. (5) for two-electron systems:  $H^-$ , He,  $Li^+$ ,  $Be^{2+}$ , and  $C^{4+}$ . The energies have converged to better than six decimal places.

TABLE VIII. Recombination rate coefficients (cm $^3$ /s) to (1  $s^2$ ) $^1$ S state from  $^2$ S and  $^2$ P states.

	$\alpha_R \times 10^{16},  \mathrm{H}^-$	$\alpha_R \times 10^{16}$ , He	$\alpha_R \times 10^{16},  \mathrm{H}^-$	$\alpha_R \times 10^{16}$ , He
T	Final state is <sup>2</sup> S state		Final state is ${}^{2}P$ state	
2000	4.36(-3)	1.93(+1)	7.35(-1)	3.37(+1)
4000	2.86(-2)	1.68(+1)	1.00	2.50(+1)
5000	5.83(-2)	1.59(+1)	1.10	2.21(+1)
7000	1.73(-1)	1.45(+1)	1.24	1.79(+1)
10000	5.07(-1)	1.32(+1)	1.35	1.40(+1)
12000	8.30(-1)	1.26(+1)	1.38	1.22(+1)
15000	1.43	1.18(+1)	1.39	1.02(+1)
17000	1.93	1.14(+1)	1.38	9.25
20000	2.59	1.09(+1)	1.36	8.07
22000	3.17	1.07(+1)	1.34	7.43
25000	3.89	1.03(+1)	1.30	6.64
30000	4.97	9.98	1.24	5.64
35000	5.86	9.55	1.18	4.89
40000	6.55	9.28	1.12	4.31
45000	7.06	9.06	1.06	3.86
50000	7.43	8.88	1.00	3.48
60000	7.81	8.62	9.04(-1)	2.91
70000	7.88	8.42	8.18(-1)	2.50
80000	7.76	8.26	7.42(-1)	2.18
90000	7.53	8.11	6.76(-1)	1.93
100000	7.25	7.97	6.19(-1)	1.73
200000	4.48	6.38	3.07(-1)	8.20(-1)
300000	2.96	4.94	1.89(-1)	5.11(-1)

### IV. CONCLUSIONS

We have calculated the photoabsorption cross sections of two-electron systems leaving the atom or ion in the  $2^{2}S$  or  $2^{2}P$  final states. In each case, the behavior with respect to increasing Z, the nuclear charge, is different. The process of ionization with excitation can take place due to the electron-electron correlations only. Therefore, this can test the quality of different theoretical methods [8]. Excitation cross sections of  $2^{2}S$  or  $2^{2}P$  states by electron impact must be augmented with the photoabsorption cross sections to infer the population of these states. We have given the ratio of the sum of these cross sections to the photoabsorption cross sections when the target is left in the  $n = 1^{2}S$  state after photoabsorption in  $H^{-}$ , He atoms, and  $Li^{+}$  ions. It should be possible to measure this ratio experimentally. Such measurements could show the relative importance of electron-electron correlation effects in

the two-electron systems. This effect is very pronounced in negative ions. We have also calculated the radiative-attachment rates for H atoms and He<sup>+</sup> ions at various electron temperatures when the final state is the  $2^{2}S$  or  $2^{2}P$  state.

Cross sections calculated here would be useful as they are needed in the investigation of astrophysical objects, the upper atmosphere, and laboratory plasmas.

As for accuracy of the calculations, all phase shifts and cross sections are converged to better than the third decimal place.

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