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Research Article

Excitation of $(1s2s)\ ^1S$, the Singlet State of Helium Atoms by Positron Impact

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Abstract. The excitation of the $(1s2s)\ ^1S$ state of a helium atom has been calculated using scattering functions obtained by the method of polarized orbitals. In this method, the distortion of each orbital is considered due to the presence of the incident particle. The distortion takes place only when the incident particle is outside the target orbital. This method has been widely used in the scattering of electrons and positrons from various targets. Plane-wave normalization of the continuum function is considered, while it has been neglected in calculations carried out by Mandal *et al*. [18], and Willis and McDowell [21]. Consequently, the present results are higher than those obtained by them.

Keywords. positron impact excitation of helium atoms

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1. Introduction and Calculations

Excitation cross sections have a wide range of applications. They are needed to analyze solar and astrophysical observations to infer the plasma parameters in various regions of the Sun and other stellar objects. Using the Maxwell distribution and excitation cross sections, rate coefficients are calculated at a particular temperature. They are then used in statistical equilibrium equations to calculate the level population of an ion under consideration and intensity ratios of various emission lines are calculated for comparison with observations. The excitation of the $(1s2s)\ ^1S$ state of a helium atom was calculated by Mandal *et al*. [18], using the *method of polarized orbitals* (MOP) [20] and by Willis and McDowell [21] using the close-coupling method. To compare the present results with those obtained in [18], we use the same approximation for calculating the scattering functions as in [18]. In the MOP, the distortion of the orbital electrons takes place only when the incident electron is outside the orbits of target electrons. However, this condition can be modified by letting the distortion take place throughout the range [6, 8], whether the incident electron or positron is inside or outside the orbits of the target electrons. This is called a hybrid theory. This has been applied in some of our previous calculations, obtaining results which agreed with the results obtained using the well-established close-coupling and R-matrix methods. We used the hybrid theory in various calculations, e.g., to calculate the excitation of $2P$ state of atomic hydrogen by electron impact [3]. Excitations to a number of ions by electron impact is discussed in a review article [9], P-wave positron-hydrogen scattering, annihilation, and positronium formation [1], the excitation of the $3D$ and $4D$ states of atomic hydrogen by electron impact [10], theory of P-wave electron-Li scattering (with one electron) elastic scattering and photo-absorption in two-electron systems [5], a recent review article on photoionization discusses photo-absorption in other systems [7]. In the present calculation, scattering functions of very high angular momenta are required. In references [18] and [21], the plane wave normalization [15] of the continuum function has not been considered, which is given by,

$$a(L) = \sqrt{4\pi(2L+1)}. \tag{1.1}$$

This normalization has been considered in all our previous publications, starting in 1977 [2], whether the continuum function refers to that of an electron scattering or of a positron scattering, as indicated in references [3, 8]. Including this normalization, cross sections for excitation are obtained and compared with those given in [18] and [21]. The continuum functions at infinity go like

$$\frac{\sin\left(kr - \frac{L\pi}{2}\right)}{k \times \text{amplitude}}, \tag{1.2}$$

where amplitude represents the amplitude of the calculated continuum function.

We write the T matrix for excitation in the form,

$$T = -\left(\frac{1}{4\pi}\right)\langle\phi_f|H_I|\phi_i\rangle. \tag{1.3}$$

The interaction Hamiltonian H_I is given by H_0-H_1, where H_0 is the Hamiltonian when the positron is far away from the helium atom, and H_1 is the Hamiltonian when the positron is close to the helium atom [2, 16],

$$H_0 = -\nabla_1^2 - \nabla_2^2 - \nabla_3^2 - \frac{2Z}{r_2} - \frac{2Z}{r_3} + \frac{2}{r_{23}}, \tag{1.4}$$

$$H_1 = -\nabla_1^2 - \nabla_2^2 - \nabla_3^2 - \frac{2Z}{r_2} - \frac{2Z}{r_3} + \frac{2}{r_{23}} + \frac{2ZN}{r_1} - \frac{2}{r_{12}} - \frac{2}{r_{13}}, \tag{1.5}$$

$$H_I = \frac{2ZN}{r_1} - \frac{2}{r_{12}} - \frac{2}{r_{13}}. \tag{1.6}$$

In eq. (1.3), ϕ_i and ϕ_f are the initial and final state wavefunctions, ϕ_i represents scattering of the positron from a helium atom with the nuclear $ZN = 2$, while ϕ_f represents the wavefunction of the excited helium atom and the outgoing wave of the positron given by

$$\phi_f(r_1; r_2, r_3) = \exp(i\vec{k}_f \cdot \vec{r}_1)\phi(r_2, r_3). \tag{1.7}$$

In the above equations, r_1 represents the positron while r_2, and r_3 represent target electrons, $r_{12} = |\vec{r}_1 - \vec{r}_2|$ and $r_{13} = |\vec{r}_1 - \vec{r}_3|$, and k_f represents the momentum of the outgoing positron.

We use Ry units: energies are in Rydberg units and lengths are in Bohr radius a_0. Therefore, cross sections are in a_0^2 units.

Cross section is given by:

$$\sigma(a_0^2) = \frac{k_f}{k_i}\int |T|^2 P_L(\Omega)d\Omega. \tag{1.8}$$

The excited $(1s2s)\ ^1S$ state wavefunction is taken from Morse *et al*. [19], where the excited state wavefunction is given by:

$$\phi(r_1,r_2) = (u_1(r_1)u(r_2) + 1 \leftrightarrow 2). \tag{1.9}$$

In the above equation,

$$u_1(r) = (\mu^3 a^2/\pi)^{0.5} e^{-\mu a r}, \tag{1.10}$$

$$u_2(r) = (\mu^5/3\pi N)^{0.5}\left[re^{-\mu r} - \left(\frac{3A}{\mu}\right)e^{-\mu b r}\right]. \tag{1.11}$$

The various quantities in equations (1.10) and (1.11) are given [19]. They are

$$a = 3.28,\ \ a\mu = 2.00,\ \ b = 2.57,\ \ b\mu = 1.57,\ \ 2\mu = 1.22, \tag{1.12}$$

$$N = 1 - 48Aa/(1+b)^4 + \frac{3A^2}{b^2}\ \text{ and }\ A = (a+b)^3/(1+a)^4. \tag{1.13}$$

Morse *et al*. [19] obtained -4.295 Ry as the energy of the $(1s2s)\ ^1S$ state. Since the ground state of helium is much lower than the excited state, the incident electron loses 1.515 Ry for exciting the $(1s2s)\ ^1S$ state.

The distorted orbitals are given by:

$$\phi(r_1;r_2,r_3) = (\varphi_0(r_2) + \epsilon(r_1,r_2)u_{1s\to p}(r_2)\cos\theta_{12}/((\pi z)^{0.5}) + [(2 \to 3)]). \tag{1.14}$$

The target function is $\varphi_0(r_2)\ \varphi_0(r_3)$, where $\varphi_0(r_2) = (z^3/\pi)^{0.5}e^{-zr_2}$.

In eq. (1.14), r_1 represents coordinate of the incident positron, and r_2, and r_3 represent coordinates of the target electrons. We are using a closed-shell target wave function which implies $z = 2 - \frac{5}{16} = 1.6875$, where 2 is the nuclear charge. In reference [20], $u_{1s\to p}(r)$ and $\epsilon(r_1,r_2)$ are given as

$$u_{1s\to p}(r) = e^{-zr}(0.5zr^2 + r), \tag{1.15}$$

$$\epsilon(r_1,r_2) = 1, \quad r_1 > r_2. \tag{1.16}$$

The step function is zero for $r_1 < r_2$. The scattering function $u(r_1)$ is obtained by:

$$\langle\varphi_0(r_2)\varphi_0(r_3)|H - E|\phi(r_1;r_2,r_3)u(\vec{r}_1)\rangle = 0. \tag{1.17}$$

The integration is over $d\Omega_1 d\vec{r}_2 d\vec{r}_3$, $E = E_0 + k^2$, where $E_0 = -2z^2$ is the target energy and k is the incident momentum, $H = H_1$, given in eq. (1.5). The equation for the continuum function by solving the equation given below:

$$\frac{d^2u}{d^2r} = \left(\frac{L(L+1)}{r^2} + V_d - 2A_{12} - k^2\right)u = 0, \tag{1.18}$$

where L is the angular momentum of the incident positron and

$$V_d = 4e^{-2zr}\left(z + \frac{1}{r}\right), \tag{1.19}$$

$$A_{12} = 4.5\left[1 - e^{-2zr}\left(4(zr)^5\frac{4}{27} + 2\frac{(zr)^4}{3} + 4\frac{(zr)^3}{3} + 2(zr)^2 + 2(zr) + 1\right)\right]\Big/(zr)^4. \tag{1.20}$$

Solving the equation for $u(r)$ for $k = 0.1$, we find the phase shift $\eta = 1.75373(-2)$ radians. This does not agree with $\eta = 3.7(-2)$ obtained in [13], using the above wave function given in eq. (1.14). In the scattering equation for the continuum function, there is a term proportional to $(9/(1.6875)^4)/r_1^4 = 1.1098\, a_0^3/r_1^4$, where 1.1098 represents the polarizability of the helium atom. To use the correct polarizability of the helium atom close to the accurately calculated polarizability in eq. (1.18), which is $1.383241\, a_0^3$ [11], we multiply the $1/r^4$ term 1.1098 by cons = 1.2463 to obtain the exact polarizability of the helium atom equal to the calculated value [11]. Now, we get phase shift $\eta = 3.419157(-2)$, which is close to the value obtained in [13].

We briefly describe the calculations carried out. We write eq. (1.3), using eq. (1.6), as

$$T = -\frac{1}{4\pi}\left\langle \phi_f \left| \frac{2ZN}{r_1} - \frac{2}{r_{12}} - \frac{2}{r_{13}} \right| \phi(r_1; r_2, r_3)u(r_1)\right\rangle, \tag{1.21}$$

where

$$\phi_f = e^{i\vec{k}_f\cdot\vec{r}_1}(u_1(r_2)u_2(r_3) + \text{exchange}). \tag{1.22}$$

The excited state functions u_1 and u_2 are given in [19]. Since the nuclear charge $ZN = 2$, we have $z = 2 - 0.3125 = 1.6875$, the closed-shell approximation for the helium atom. We write some of the various term in eq. (1.21) in the form given below:

$$T_1 = \frac{1}{\pi}\left\langle \phi_f \left| \frac{1}{r_1} \right| \phi(r_1; r_2, r_3)\right\rangle, \tag{1.23}$$

$$T_1 = T_{11} + T_{12} + T_{13} + T_{14}, \tag{1.24}$$

$$T_{11} = -\frac{4}{\sqrt{2}}(I_1 I_2 + I_2 I_1)J_1. \tag{1.25}$$

In the above equation,

$$I_1 = 4(\mu a z)^{1.5}/(\mu a z)^3, \tag{1.26}$$

$$I_2 = 24(\mu^5 z^3/3N)^{0.5}\left(1/(\mu + z)^4 - \frac{A}{\mu}\frac{1}{(\mu b + z)^3}\right) \tag{1.27}$$

and

$$J_1 = \int j_L(k_f r)u(r)dr, \tag{1.28}$$

where j_L is the spherical Bessel function of an angular momentum L, and

$$T_{12} = 0 = T_{13} = T_{14}, \tag{1.29}$$

$$T_{21} = \frac{1}{2\pi}\frac{1}{\sqrt{2}}\int e^{-ik_f\cdot r}(u_1(r_2)u_2(r_3) + 2 \leftrightarrow 3)\left|\frac{1}{r_{12}} + \frac{1}{r_{13}}\right| v_0(r_2)v_0(r_3)u(r_1)d\vec{r}_1 d\vec{r}_2 d\vec{d}_3, \tag{1.30}$$

$$T_{21} = \frac{16\pi}{2\sqrt{2}}(I_2 J_2 + I_1 J_3), \tag{1.31}$$

where

$$J_2 = \int j_L(k_f r)X_1((r)u(\vec{r})d\vec{r}, \tag{1.32}$$

$$J_3 = \int j_L(k_f r)X_2(r)u(\vec{r})d\vec{r}, \tag{1.33}$$

where

$$X_1(r_1) = \int \frac{u_1(r_2)}{r_{12}} v_0(r_2) d\vec{r}_2 , \tag{1.34}$$

$$X_2(r_1) = \int \frac{u_2(r_2)}{r_{12}} v_0(r_2) d\vec{r}_2 , \tag{1.35}$$

$$T_{22} = T_{21} , \tag{1.36}$$

$$T_{23} = \frac{2}{3(2z\pi)^{0.5}} \int e^{-ik_f \cdot r} (u_1(r_2) I_2 + u_2(r_2) I_1) | \frac{r_<}{r_>^2} \left| \frac{\epsilon(r_1,r_2)}{{r_1}^2} \right| u_{1s\to p}(r_2) u(r_1) d\vec{r}_1 r_2^2 dr_2, \tag{1.37}$$

where

$$u_{1s\to p}(r)(r) = e^{-zr}(0.5zr^2 + r). \tag{1.38}$$

In the above equations $X_1(r)$ and $X_2(r)$ are complicated functions of the coordinate r, therefore, only the integral form is given. Moreover, we have not given all the various components of T matrix.

$$T_{24} = T_{23} , \tag{1.39}$$

$$\text{cross section } (a_0^2) = (4 \times 3.14159)(2L+1) \frac{k_f}{k} \int |T|^2 P_L(\Omega). \tag{1.40}$$

2. Results

In Table 1, we give the cross sections for excitation of the helium atom at various energies.

In Table 2, we give convergence of cross sections $\sigma(a_0^2)$ with the angular momentum L at $E = 60.0$ eV.

Table 1. Cross sections $\sigma(a_0^2)$ of the excitation of the $(1s2s)$ ^1S state of helium

E (eV)	With the normalization given in eq. (1.1)	Without the normalization as given in [18]
40.0	1.239	0.1200
50.0	1.620	0.1060
60.0	1.927	0.0946
80.0	2.707	0.0757
100.0	2.914	0.0631
150.0	3.407	0.0437
200.0	3.248	0.0336

Table 2. Convergence of the cross section $\sigma(a_0^2)$ at 60.0 eV with increasing Lm, the maximum L

Lm	$\sigma(a^2)$	Lm	$\sigma(a^2)$
0	0.1402	10	1.8872
1	0.3771	11	1.9032
2	0.6889	12	1.9139
3	1.0174	13	1.920
4	1.2988	14	1.9196
5	1.5081	15	1.9250
6	1.6560	16	1.9261
7	1.7536	17	1.9266
8	1.8191	18	1.9268
9	1.8602	19	1.9268

In Table 3, we give phase shifts for a few angular momenta L of the incident positron with energy 40 eV.

We give convergence of the cross sections and phase shifts with increasing L so that the future workers might be able to compare their results with those obtained in the present calculations. Coleman *et al*. [14] have measured the excitation of the excited $(1s2s)$ ^1S state

Table 3. Phase shifts (radians) for the incident energy 40 eV for various values of L

L	Phase shift	L	Phase shift
0	−0.37238	5	0.00957
1	−0.01426	6	0.00589
2	0.03672	7	0.00384
3	0.02758	8	0.00263
4	0.01631	9	0.00188

of helium by positron impact. Mandal *et al*. [18] find a reasonable agreement with their results when the plane wave normalization was neglected. In the present work, inclusion of the normalization gives higher cross sections, and therefore, no agreement between the experimental [14] and theoretical results [18, 21] is obtained. It is not clear how the measured cross sections were normalized.

3. Conclusions

In [18], calculations have been carried out for the excitation of a helium atom by positron impact by using the *Method of Polarized Orbitals* (MOP) [20]. The present calculations have also been carried out in the same approximation (MOP) to compare the present results with those of [18]. The results obtained do not agree with those given in [18] nor with the experimental results [14] when normalization of the continuum function is included. Mandal *et al*. [18] and Willis and McDowell [21] obtained agreement with the experimental results [14] because of the neglect of the plane normalization [15] of the continuum function. It is not clear why the normalization was neglected by authors of references [18] and [21], and how the experimental results were normalized. The main object of this study is to point out the neglect of the normalization of the continuum functions $a(L) = \sqrt{4\pi(2L+1)}$.

In the excitation of $2S$ state of hydrogen by electron impact [4], we included the normalization of the continuum functions $a(L) = \sqrt{4\pi(2L+1}$. Our results for exciting the $2S$ state [4] agree with those obtained by Burke *et al*. [12] using the close-coupling formalism. Furthermore, our results agree with the experimental results of Kauppilla *et al*. [17]. If we had not included the normalization, there would have been no agreement with the results of references [12] and [17]. In reference [4], the excitation is from the $1S$ state to the $2S$ state. Now, we have are dealing with the excitation of the $(1s1s)$ state to the $(1s2s)$ state. The formalism is the same in both cases and physics cannot be different in these two processes.

It is not possible for us to know the experimental details to infer as to why there is an agreement of results obtained in references [18] and [21], without considering the normalization of the continuum functions, with observations.

Competing Interests

The author declares that he has no competing interests.

Authors' Contributions

The author wrote, read and approved the final manuscript.

References

[1] A. K. Bhatia, P-wave positron-hydrogen scattering, annihilation, and positronium formation, *Atoms* **5**(2) (2017), 17, DOI: 10.3390/atoms5020017.

[2] A. K. Bhatia, and A. A. Temkin, A distorted-wave methodology for electron-ion impact excitation: calculation for two-electron ions, *Journal of Physics B: Atomic and Molecular Physics* **10**(14) (1977), 2893, DOI: 10.1088/0022-3700/10/14/022.

[3] A. K. Bhatia, Excitation of the $2P$ state of atomic hydrogen by electron impact, *Atoms* **10**(4) (2022), 113, DOI: 10.3390/atoms10040113.

[4] A. K. Bhatia, Excitation of the $2S$ state of atomic hydrogen by electron impact, *Atoms* **6**(1) (2018), 7, DOI: 10.3390/atoms6010007.

[5] A. K. Bhatia, Hybrid theory of P-wave electron-Li^{2+} elastic scattering and photoabsorption in two-electron systems, *Physical Review A* **87** (2013), 042705, DOI: 10.1103/PhysRevA.87.042705.

[6] A. K. Bhatia, Hybrid theory of electron-hydrogen scattering, *Physical Review A* **75** (2007), 032713, DOI: 10.1103/PhysRevA.75.032713.

[7] A. K. Bhatia, Photoejection from various systems and radiative-rate coefficients, *Atoms* **10**(1) (2022), 9, DOI: 10.3390/atoms10010009.

[8] A. K. Bhatia, Scattering, and its applications to various atomic processes: elastic scattering, resonances, photoabsorption, Rydberg states, and opacity of the atmosphere of the Sun and stellar objects, *Atoms* **8**(4) (2020), 78, DOI: 10.3390/atoms8040078.

[9] A. K. Bhatia, Superstructure and distorted-wave codes and their applications, *Atoms* **10**(2) (2022), 47, DOI: 10.3390/atoms10020047.

[10] A. K. Bhatia, The excitation of the $3D$ and $4D$ states of atomic hydrogen by electron impact, *Atoms* **11**(10) (2023), 139, DOI: 10.3390/atoms11100136.

[11] A. K. Bhatia and R. J. Drachman, Polarizability of helium and negative hydrogen ion, *Journal of Physics B: Atomic, Molecular and Optical Physics* **27** (1994), 1299, DOI: 10.1088/0953-4075/27/7/005.

[12] P. G. Burke, H. M. Shey and K. Smith, Collision of slow electrons and positrons with atomic hydrogen, *Physical Review Journals Archive* **129** (1963), 1258, DOI: 10.1103/PhysRev.129.1258.

[13] R. I. Campeanu and J. W. Humberston, The scattering of s-wave positrons by helium, *Journal of Physics B: Atomic and Molecular Physics* **10** (1977), L153, DOI: 10.1088/0022-3700/10/5/007.

[14] P. S. Coleman and J. T. Hutton, Excitation of helium atoms by positron impact, *Physical Review Letters* **25** (1980), 3017, DOI: 10.1103/PhysRevLett.45.2017.

[15] A. R. Edmonds, *Angular Momentum in Quantum Mechanics*, Princeton University Press, Princeton, 146 pages (1957).

[16] C. J. Joachain, *Quantum Collision Theory*, North-Holland Publishing Company, Amsterdam – Oxford, 710 pages (1975).

[17] W. E. Kauppilla, W. R. Ott and W. L. Fite, Excitation of atomic hydrogen in the metastable $2^2S_{\frac{1}{2}}$ state by electron impact, *Physical Review A* **1** (1970), 1099, DOI: 10.1103/PhysRevA.1.1099.

[18] S. K. Mandal, M. Basu and A. S. Ghosh, Positron-impact excitation of helium, *Physical Review A* **33** (1986), 727, DOI: 10.1103/PhysRevA.33.727.

[19] P. M. Morse, L. A. Young and E. S. Haurwitz, Tables for determining atomic wave functions and energies, *Physical Review Journals Archive* **48** (1935), 948, DOI: 10.1103/PhysRev.48.948.

[20] A. Temkin, A note on the scattering of electrons from atomic hydrogen, *Physical Review Journals Archive* **116** (1959), 358, DOI: 10.1103/PhysRev.116.358.

[21] S. L. Willis and M. R. C. McDowell, Pseudo states effects on positron-helium excitation cross sections at intermediate energies, *Journal of Physics B: Atomic and Molecular Physics* **15**(1) (1982), L31, DOI: 10.1088/0022-3700/15/1/007.