Excitation of the n^1S States of Helium by Proton Impact

William J. B. Oldham, Jr.
National Aeronautics and Space Administration, Manned Spacecraft Center, Houston, Texas
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The first Born-approximation cross sections for proton excitation of helium from the ground state to the n^1S ($n=4$ to 7) states are calculated using a 53-term correlated ground-state wave function and 40-term correlated wave functions for the excited states. Generalized oscillator strengths for the respective transitions are also given. The results are compared with the only previous theoretical calculation and with existing experimental values. The agreement between theory and experiment is poor for absolute values, but the curves obtained from $\log\sigma$ vs $\log E$ plots have the same slope at large impact energies.

INTRODUCTION

In a recent paper, Thomas and Bent[1] (hereafter referred to as TB) report new results of experimental measurements of the excitation cross sections of neutral helium from the ground state to the n^1S ($n=4$ to 7) states by 0.15- to 1-MeV proton impact, and summarize previous experimental results. In a second paper, Thomas[2] reviews the theoretical picture and points out that the only theoretical predictions for these cross sections are those scaled by Gaillard[3] from electron-impact calculations by Fox.[4] In his calculations, Fox used products of one-electron orbitals to approximate the various states of helium. Although the resulting theoretical values of Gaillard are within the error bounds reported in TB, the agreement between theory and experiment is poor. Furthermore, significant differences exist between the data of the several different recently reported experiments.[5-8] For instance, consider the data of Van den Bos *et al.*[7] Since the cross sections are reported for proton energy only up to 0.15 MeV, the range of overlap of this experiment with that of TB is small. However, the cross sections at 0.15 MeV differ by approximately a factor of 2, and it is clear that the two experiments do not agree. In view of these discrepancies and the inadequacy of the wave functions used in the only previous calculation, it is important to recalculate the cross sections and generalized oscillator strengths in the Born approximation with accurate correlated wave functions. The purpose of this paper is to present such results.

An accurate 53-term Hylleraas-expansion wave function is available for the ground state of helium,[9] and 40-term Hylleraas expansions are available for the 4^1S-7^1S states.[10] These functions are used here to evalute the relevant Born matrix elements. In addition, cross sections are given with the ground-state wave function approximated by the Hylleraas six-parameter wave function.[11] It is found that the cross sections differ only by about 1.5% (in the worst case) depending on which ground-state wave function is used. In spite of the accuracy of the wave functions, the cross sections obtained do not agree well in absolute value with the experimental results of TB.

CALCULATIONS

The first Born approximation of the cross section for excitation of helium from the ground state ψ_0 to the state ψ_n by proton impact is given by (in units of πa_0^2)

$$\sigma_{0n} = 32\mu^2 K_0^{-2} \int_{K_{\min}}^{K_{\max}} |I(K)|^2 K^{-3} dK. \tag{1}$$

$\vec{K} = \vec{K}_0 - \vec{K}_n$ is the momentum change vector, where $\vec{K}_0$ and $\vec{K}_n$ are, respectively, the initial and final wave vectors of relative motion. K_n is determined by the conservation of energy equation

$$K_0^2 = K_n^2 + 2\mu E_n,$$

and μ is the reduced mass of the two-body system with E_n the excitation energy of the nth state measured from the ground state. $K_{\min} = K_0 - K_n$ and $K_{\max} = K_0 + K_n$. $I(K)$ is the Born matrix element

$$I(K) = \int e^{i\vec{K}\cdot\vec{r}_1} \psi_n^*(\vec{r}_1, \vec{r}_2)\psi_0(\vec{r}_1, \vec{r}_2) d\vec{r}_1 d\vec{r}_2 \tag{2}$$

in which $\vec{r}_i$ denotes the radius vector of the ith electron measured from the helium nucleus. The generalized oscillator strength, f_{0n}, for the transition from the ground state to the nth state is defined by[12]

$$f_{0n} = 4E_n |I(K)|^2 K^{-2}/R , \tag{3}$$

where R is the Rydberg energy.

The evaluation of the matrix element of Eq. (2) is a straightforward but tedious task and can be done analytically. The evaluation of the function in Eq. (3) and the final integration over the momentum change variable of Eq. (1) must be done numerically.

In general, and in particular for the S-S transitions considered here, the wave functions ψ_0 and ψ_n should be orthogonal. The overlap integrals for the wave functions used in these computations are

TABLE I. Normalization and overlap integrals.

Ground state	Ground state normalization	4^1S	5^1S	6^1S	7^1S
6 Parameter	1.3808[11]	-2.4×10^{-2}	-1.7×10^{-2}	-1.2×10^{-2}	-1.0×10^{-2}
53 Term	0.59297[9]	1.0×10^{-5}	$7.\ \times 10^{-6}$	4.9×10^{-6}	5.0×10^{-6}
Normalization excited states		2.0666×10^{-3}	6.2261×10^{-4}	2.2530×10^{-4}	1.2747×10^{-4}

listed in Table I. As can be seen, the 53-term ground-state and any one of the 40-term excited-state wave functions have a small overlap. The corresponding overlap of the six-parameter wave function with any one of the excited-state functions is considerably larger. In Table II, the experimental values of the energies[13] of the various states are compared with the corresponding energies given for those states derived by use of the above referenced wave functions. It is seen that the energy eigenvalues are predicted quite accurately through the use of these wave functions. Because of the accuracy and length of these wave functions, it does not seem reasonable to try to orthogonalize them by a projection process. Such a process would certainly ruin one or the other of the wave functions. The nonzero overlap only appreciably affects the generalized oscillator strengths for small values of the magnitude of the momentum-change vector, and thereby only contributes to the excitation cross section for these same values. It is possible to reduce this contribution for small K by expanding $\exp(i\vec{K}\cdot\vec{r})$ of the matrix element in a power series. The first term of $I(K)$ is then just the overlap integral J. We then set $J=0$ and compute the first several nonzero terms in the expansion until the desired accuracy is obtained. The Born matrix element is written as

$$I(K)=\sum_{l=1}[(iK)2^l/2l\,!]c_l\ , \tag{4}$$

where

$$c_l=\int d\vec{r}_1\,d\vec{r}_2\psi_n{}^*(\vec{r}_1,\vec{r}_2)\psi_0(\vec{r}_1,\vec{r}_2)r_1{}^{2l}\cos^{2l}\theta_1 .$$

The generalized oscillator strength is written as

$$f_{0n}(K)=\alpha K^2\left(\sum_{l=1}c_l i^{2l}K^{2l-2}\right)^2 , \tag{5}$$

where $\alpha=256\pi^4E_nN_0{}^2N_n{}^2/R$. N_0 and N_n are, respectively, the normalization coefficients of the ground-state and excited-state wave functions. This method was used to compute the generalized oscillator strengths and the cross sections over the range $K=K_{\min}$ to $K=0.5$.

In calculations of this type, it is customary to give the results of the oscillator strengths and cross sections from both the so-called "length" and "velocity" formulas. In this work, only the "length" formula has been used. Results quoted by Kim[14] for the generalized oscillator strengths for the transition -2^1S with the same ground state as used here and the 54-term excited-state wave function of Weiss[9] show a discrepancy of only 0.5% between the "length" and "velocity" formulas. Similarly the discrepancy for the 1^1S-3^1S transition is only 1.5%. In a recent paper by Bell, *et al.*,[15] on the excitation cross sections, 1^1S-N^1P, in which less accurate wave functions than those used here are utilized, the variation of "length" and "velocity" formula is only 4%. In view of the large experimental discrepancies and the discrepancies between these calculations of this work and the experimental values, it is not felt that an unexpectedly large variation of even 4% between "length" and "velocity" results would add anything new. In fact, judging from the variations quoted above, one would not expect the "length"-"velocity" variation to be even as great as 4%.

TABLE II. Total energies (in atomic units) for various n^1S of neutral helium.

	1^1S	4^1S	5^1S	6^1S	7^1S
53-term ground state	2.90372				
40-term[10] excited state		2.0336	2.0212	2.0145	2.0106
Experimental[13]	2.90372	2.0337	2.0213	2.0147	2.0108

RESULTS AND DISCUSSION

The results for the generalized oscillator strengths, Eq. (3), are given in Table III. For

TABLE III. Generalized oscillator strengths $\times 10^4$ for n^1S excitation.

K^2 (atomic units)	4^1S	5^1S	6^1S	7^1S
0.0625	3.72	1.80	1.00	0.652
0.140625	7.77	3.76	2.11	1.37
0.25	12.4	6.04	3.39	2.21
0.5625	20.5	10.1	5.68	3.71
1.0	23.6	11.7	6.65	4.37
1.5625	21.6	10.8	6.17	4.06
2.25	16.8	8.50	4.87	3.208
3.0625	11.9	6.02	3.45	2.28
4.0	7.82	3.99	2.29	1.52
6.250	3.10	1.59	0.915	0.606
7.5625	1.92	0.986	0.568	0.377

TABLE IV. Expansion coefficients for Eq. (5).

Term	C_1	C_2	C_3	C_4	C_5
4^1S	0.31130	0.145	0.0116	−0.0275	−0.024
5^1S	0.7117	0.3139	0.010	−0.070	−0.055
6^1S	1.4635	0.626	0.0042	−0.15	−0.011
7^1S	2.08	0.847	0.0074	−0.22	−0.016

$K \leq 0.5 (K^2 \leq 0.25)$, Eq. (5) was used to compute the generalized oscillator strengths. The first five expansion coefficients needed to compute the oscillator strength from Eq. (5) are given in Table IV with the required normalization coefficients given in Table I.

The cross sections computed from Eq. (1) are given in Table V. The Born matrix element was computed in three ways, all with the 40-term excited-state wave functions; (a) with the six-parameter ground-state wave function in Eq. (2), (b) with the 53-term ground-state wave function in Eq. (2), and (c) with the 53-term wave function in the expansion method for the integration from $K=(K_{\min}, \frac{1}{2}$ and the same ground state in Eq. (2) for the integration for $K=(\frac{1}{2}, K_{\max})$. It can be seen that the six-parameter wave function is adequate for the cross sections except at the highest impact energies. This is to be expected since at higher impact energies it is necessary to integrate over small momentum transfer, and it is at small momentum transfer that the overlap integral contributes to the cross section. At higher impact energies than 2 MeV, the six-parameter wave function would yield unreliable cross sections. The 53-term ground-state wave function gives reliable results in most cases up to 2 MeV. Beyond this, it would be essential to use the expansion method to compute the cross section even though the 53-term function has a small overlap with the excited-state wave functions. A rough idea of the importance of the size of the overlap integral J can be ascertained from Eq. (4). If $J \neq 0$, then the first term in the expansion in Eq. (5) is J/K^2, which must then be compared with the first expansion coefficient, c_1, given in Table IV. If J/K^2 is appreciably compared to c_1 for values of K in the range of integration, then Eq. (4) should be used to compute the Born matrix element instead of Eq. (2). For $J/K^2 \approx 10^{-3} c_1$, $K = 0.18$. The lower limit of integration $K_{\min}$ is equal to 0.097 for 2-MeV incident protons. The relatively good results (as compared with the expansion method) shown in Column 1 of Table V are obtained because the low-momentum transfer does not contribute heavily to the cross section. For the six-parameter wave function, fairly good results are obtained because the small momentum transfers do not add greatly to the cross section and possibly because of the averaging effects of the integral in Eq. (1).

TABLE V. n^1S excitation cross sections for He by proton impact.

Proton energy lab system MeV	Term	$\sigma(10^{-4}\pi a_0^2)$ 53-term ground state	$\sigma(10^{-4}\pi a_0^2)$ Eq. (4) used for $K_{\min}-\frac{1}{2}$	$\sigma(10^{-4}\pi a_0^2)$ Six-parameter ground state
0.25	4_1S	14.6	14.6	14.5
	5^1S	7.11	7.11	7.06
	6^1S	3.99	4.00	3.95
	7^1S	2.59	2.59	2.59
0.50	4^1S	7.53	7.54	7.52
	5^1S	3.68	3.68	3.65
	6^1S	2.07	2.07	2.05
	7^1S	1.34	1.34	1.34
1.0	4^1S	3.83	3.84	3.82
	5^1S	1.87	1.87	1.86
	6^1S	1.05	1.05	1.04
	7^1S	0.686	0.686	0.678
2.0	4^1S	1.93	1.94	1.93
	5^1S	0.942	0.945	0.935
	6^1S	0.530	0.531	0.523
	7^1S	0.346	0.346	0.341

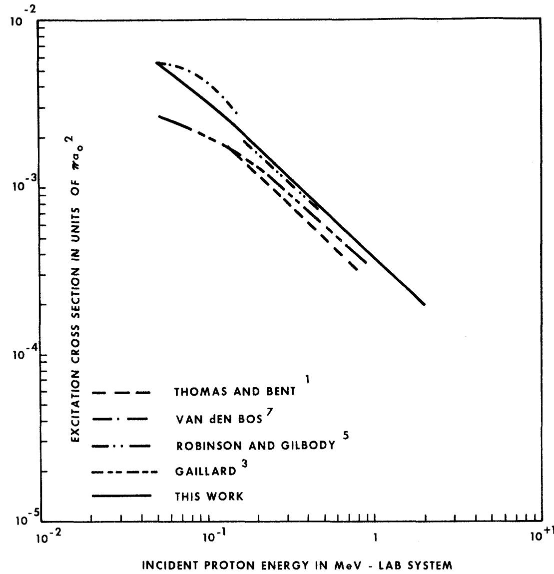

FIG. 1. Excitation cross sections 1^1S–n^1S of He by proton impact.

In Fig. 1, the log of σ_{0n} as obtained in this work is plotted vs the log of E, the proton-impact energy, along with the experimental values of TB. It can be readily seen that the agreement in absolute values is poor. However, the two sets of curves do appear to have the same slopes at the larger impact energies. Using the data of TB over the range of $E = 0.2–0.9$ MeV, the slope of a least-squares straight line is -0.99. From the two theoretical points at $E = 0.5$ and 2.0, one obtains -0.98 for the slope of the theoretical curve. Hence, the two slopes agree to about 1%.

In Fig. 2, the case for 4^1S excitation is shown. The recent data of Denis *et al.*[6] are not shown on the figure since they are in essential agreement with those of TB. The theoretical values of Gaillard[3] are in better absolute agreement with the experimental values than those of this work, but his curves appear to have the wrong slope at large impact energies. It appears that all of the experimental curves have the same slope at large impact

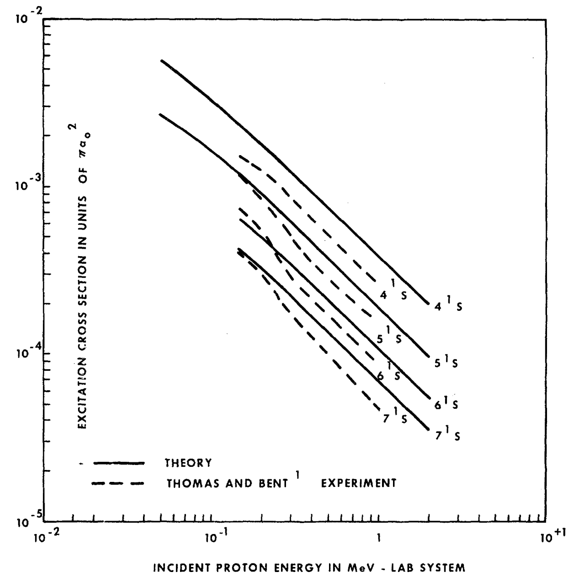

FIG. 2. Excitation cross sections 1^1S–4^1S of He by proton impact.

energies, but different absolute values; hence, the experimental curves could be normalized to the values of this work with resulting over-all agreement over a wide range of impact energies. However, such a procedure requires a great deal of freedom with the experimental data, and it is not clear what it would prove.

CONCLUSIONS

Since the experimental data have such a spread of values, it is impossible at this time to adequately appraise the cross sections computed in this work. However, if the experimental data of TB and Denis *et al.* stand up under further experimental observations, then the disagreement found here would represent a notable failure of the Born approximation.

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