

## Elastic and Inelastic Scattering of Electrons from the $S$ States of Atomic Hydrogen\*

KENNETH SMITH

Argonne National Laboratory, Argonne, Illinois

(Received May 19, 1960; revised manuscript received August 1, 1960)

Total elastic and inelastic cross sections for the scattering of electrons (including exchange) from the  $1s$ ,  $2s$ , and  $3s$  states of atomic hydrogen have been calculated in three approximations using the method of partial waves. The purpose of this report is to present the  $S$ -,  $P$ -, and  $D$ -wave contributions to the elastic,  $Q_{1s-1s}$ , and inelastic,  $Q_{1s-2s}$ , cross sections.

### INTRODUCTION

THE discrepancy between the experiments of Beder-son, Malamud, and Hammer<sup>1</sup> and of Brackman, Fite, and Neynaber<sup>2</sup> on the cross section for the elastic scattering of electrons by hydrogen atoms in the  $1s$  state has given a new impetus to wave mechanical investigations of this problem. Further uncertainty has been introduced into this problem by the different experimental results of Lichten and Schultz<sup>3</sup> and Stebbings *et al.*<sup>4</sup> in measuring the inelastic cross section for the excitation of the  $2s$  state of atomic hydrogen by electron impact. The former authors normalized their results to the Born approximation at 40 eV, while the latter performed a measurement relative to  $Q_{1s-2p}$ .

The uncertainty presently existing in the problem has emphasized the need for calculations which make as few approximations as possible. The purpose of the present paper is to examine the contributions to the cross sections from  $P$  and  $D$  partial waves and the effect of  $S$ -state distortion. Electron exchange has been taken into account.

A brief description of the theory employed is given in Sec. 1. The inelastic scattering results are presented in Sec. 2 where they are compared with other calculations and experiments, the elastic scattering results are presented in Sec. 3.

All cross sections are given in units of  $\pi a_0^2$ .

### 1. THEORY

The usual procedure in wave mechanical scattering problems is to separate out the motion of the projectile and target by expanding the total wave function for the system (which should be symmetrized in accordance with the Pauli exclusion principle) in terms of the complete set of eigenfunctions of the target Hamiltonian. The number of terms taken in this expansion determines the approximation one is working in. The resulting systems of coupled second-order integro-differential

equations for the expansion coefficients must be solved for the asymptotic parameters required to calculate the cross sections.

The name "one-body exchange approximation" is given to the approximation which assumes that only one state need be taken in the eigenfunction expansion. McEachran and Fraser<sup>5</sup> have calculated the  $Q_{1s-1s}$  elastic scattering cross section in this approximation for  $l \leq 2$  partial wave contributions. Their results have been used to check the present method.

The "strong-coupling exchange approximation" pertains when two terms are believed to be an adequate approximation to the total wave function. Marriott<sup>6</sup> has used this approximation in the electron-hydrogen atom problem assuming  $1s$  and  $2s$  coupling. However, Marriott only calculated the  $l=0$  contribution to the cross sections. In the present paper, Marriott's calculations have been checked and extended to include  $l=1$  and  $l=2$  contributions.

In the present work, some results are reported for the "three-term exchange approximation" in which the eigenfunction expansion is assumed to be given by  $1s$ ,  $2s$ , and  $3s$  states. In this way it is possible to examine the effect of  $S$ -state distortion on both the elastic and inelastic cross sections. This effect has been examined by Smith, Miller, and Mumford<sup>7</sup> in this approximation, but neglecting exchange effects.

The systems of coupled second-order integro-differential equations which are to be solved on the computing machine are well known; see Massey.<sup>8</sup> A straightforward iterative method was used to calculate the desired asymptotic parameters. In the first iteration, the integral terms were neglected and the remaining differential equations were integrated as an initial-value problem. The phase shifts and amplitudes thus obtained were considered as first approximations, while the solutions of the equations were substituted into the integral terms to get a first approximation to these functions. The system of differential equations was again solved, now including the approximate integral terms. This proce-

\* This work was performed under the auspices of the U. S. Atomic Energy Commission.

<sup>1</sup> B. Beder-son, H. Malamud, and J. Hammer, *Bull. Am. Phys. Soc.* **2**, 172 (1957).

<sup>2</sup> R. T. Brackman, W. L. Fite, and R. H. Neynaber, *Phys. Rev.* **112**, 1157 (1958).

<sup>3</sup> W. Lichten and S. Schultz, *Phys. Rev.* **116**, 1132 (1959).

<sup>4</sup> R. F. Stebbings, W. L. Fite, D. G. Hummer, and R. T. Brackmann, General Atomic Report GA-339, April 22, 1960 (unpublished).

<sup>5</sup> R. P. McEachran and P. A. Fraser, *Can. J. Phys.* **38**, 317 (1960).

<sup>6</sup> R. Marriott, *Proc. Phys. Soc. (London)* **72**, 121 (1958).

<sup>7</sup> K. Smith, W. F. Miller, and A. J. P. Mumford, *Proc. Phys. Soc. (London)* (to be published).

<sup>8</sup> H. S. W. Massey, *Handbuch der Physik* edited by S. Flügge (Springer-Verlag, Berlin, 1956), Vol. 36, p. 372.

TABLE I. Partial wave contributions to the inelastic cross sections for the scattering of electrons from hydrogen atoms:  $Q_{1s-2s}$ . Row (a) corresponds to 1s-2s coupling; row (b) corresponds to 1s-2s-3s coupling. The numbers in square brackets are those of Marriott.<sup>a</sup> The numbers in parenthesis have been included to show the extent to which the reciprocity condition has been satisfied (a check on the numerical accuracy), i.e., (a)  $\equiv (|k_0^2 Q_{1s-2s} - k_1^2 Q_{2s-1s}|)$ . The statistical factors of  $\frac{1}{2}$  and  $\frac{3}{4}$  are included. The plus and minus signs correspond to symmetric and antisymmetric spatial wave functions, respectively.

$l$	ev	11.0		13.6		19.6		30.6	
		+	-	+	-	+	-	+	-
0	(a)	0.0384 [0.0383] (0.0022)	0.0 [0.0] (0.0003)	0.0714 [0.072] (0.0)	0.0027 [0.0021] (0.003)	[0.0547]	[0.0061]	0.0238 [0.0242] (0.011)	[0.0073]
	(b)			0.0443 (0.0017)				0.0233 (0.0003)	0.0069 (0.0002)
1	(a)	0.008 (0.025)	0.1736 (0.003)	0.051 (0.028)	0.161 (0.011)	0.053 (0.0036)	0.0735 (0.0033)	0.0383 (0.0)	0.0358 (0.0013)
	(b)			0.045 (0.0004)	0.1197 (0.0013)			0.0369 (0.0001)	0.0334 (0.0)
2	(a)			0.0 (0.0)	0.046 (0.013)	0.0053 (0.0)	0.0577 (0.0003)	0.011 (0.0025)	0.040 (0.0033)
	(b)							0.0389 (0.0004)	

<sup>a</sup> See reference 6.

ture was continued until the asymptotic parameters obtained in the  $(i+1)$  iteration were the same as those of the  $(i)$  iteration to within a given epsilon. Further details of the method can be found in the report by Cody and Smith.<sup>9</sup>

## 2. INELASTIC SCATTERING

The inelastic scattering cross sections,  $Q_{1s-2s}$ , are presented in Table I.

The first point to note in Table I is that the present method reproduces Marriott's (noniterative) results to three decimal places. The second point is that in both

the 1s-2s approximation, row (a), and the 1s-2s-3s approximation, row (b), the  $l > 0$  contributions are very important.

The effect of the 3s state on the  $Q_{1s-2s}$  cross section becomes increasingly important with decreasing energy, the effect tending to decrease the cross section from the values obtained by the strong-coupling approximation. We note that the total cross section at 30 ev, as calculated here, agrees quite well with the Born approximation. This result tends to support Lichten and Schultz<sup>3</sup> in normalizing their experimental results at energies between 30 and 40 ev, although it must be emphasized that nonspherical distortion of the hydrogen atom has been neglected in all results reported here. The total inelastic cross section is plotted as a function of energy in Fig. 1.

## 3. ELASTIC SCATTERING

The elastic scattering cross sections,  $Q_{1s-1s}$ , are given in Table II.

In Table II it is seen that the 3s state has negligible influence on  $Q_{1s-1s}$ . Indeed, on comparing the results of Table II with the one-body exchange approximation of McEachran and Fraser<sup>5</sup> it is seen that even the 2s state has only a slight effect on this cross section. It is also noted that although the  $l > 0$  contributions are significant, they are not so important as in the corresponding inelastic case.

Detailed comparison of the calculated values reported here with the experimental results<sup>1,2</sup> is not possible since the experiments were performed at energies below those given in Table II. However, from Table II it is seen that the  $l=2$  (i.e.,  $d$  wave) contributions decrease in importance with decreasing energy. One might expect this tendency to continue down into energies below the excitation thresholds. To make a definite statement, calculations would have to be carried out at the low energies

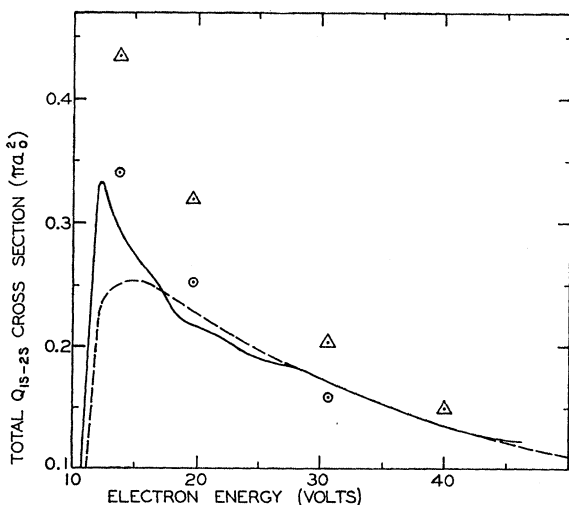


FIG. 1. Total cross section for the excitation of H(2s) by electron impact. Solid line: Lichten and Schultz<sup>3</sup>; dotted line: Born approximation<sup>3</sup>;  $\Delta$ : Smith, Miller, and Mumford<sup>7</sup>;  $\circ$ : present calculation for  $l \leq 2$ , and 1s-2s coupling.

<sup>9</sup> W. J. Cody and K. Smith, Argonne National Laboratory Report ANL-6121 (unpublished).

TABLE II. Partial wave contributions to the elastic cross sections for the scattering of electrons from hydrogen atoms:  $Q_{1s-1s}$ . Rows (a) and (b) have the same significance as in Table I.

$l$ \ $ev$	11.0		13.6		19.6		30.6	
	+	-	+	-	+	-	+	-
0 (a)	0.4358	3.6873	0.2856	2.8954			0.088	
(b)	[0.4309]	[3.68315]	[0.2828]	[2.90303]	[0.1397]	[1.8294]	[0.0904]	[0.9714]
			0.2803				0.0898	0.9678
1 (a)	0.046	1.3768	0.0333	1.15737	0.0107	0.815	0.0012	0.4855
(b)			0.0306	1.1586			0.0012	0.4835
2 (a)			0.0014	0.0565	0.0005	0.068	0.0	0.0718
(b)								0.0722

taking into account virtual excitation of the atomic levels.

#### 4. DISCUSSION AND CONCLUSIONS

It is conceivable that there exists some programming error in the method used to calculate the cross sections reported here. This seems unlikely since the method reproduces, to two decimal places, the  $l=0, 1$ , and 2 results of McEachran and Fraser<sup>5</sup> at  $k_0a_0=0.9$  and 1.0 and the  $l=0$  results of Marriott,<sup>6</sup> see Tables I and II. Furthermore, after the phase shifts and amplitudes have been calculated, the cross sections were calculated by two different methods: (a) using the explicit formulas, see for example Marriott,<sup>6</sup> and (b) using the matrix method of Smith.<sup>10</sup> Following Bransden and McKee,<sup>11</sup> the relation

$$k_0^2 Q_{1s-2s} - k_1^2 Q_{2s-1s} = 0$$

was used as a test of numerical errors. How well this relation was satisfied has been shown in Table I by the numbers in parenthesis. Using this test suggests that the method is most accurate at the higher energies and that the cross sections reported here are accurate to two decimal places. The accuracy could have been improved by using double-precision arithmetic in the Runge-

Kutta-Gill<sup>12</sup> scheme for integrating the differential equations and by increasing the number of mesh points in performing the integrals. However, since  $P$  and  $D$  states were neglected in the eigenfunction expansion, it is felt not worth while to use additional computer time in improving the accuracy within the framework of the present formulation, but rather the problem should be reformulated in the representation suggested by Percival and Seaton.<sup>13</sup>

In conclusion, if the number of terms required in the eigenfunction expansion can be considered as a measure of the distortion of the target atom, then the results of the present work indicate that  $S$ -state distortion is unimportant when calculating elastic cross sections, but is quite important for inelastic cross sections at energies just above threshold. Since the present calculations of  $Q_{1s-2s}$  are several times bigger than the experimental results of Stebbings *et al.*,<sup>4</sup> it is quite imperative that  $P$ - and  $D$ -distortive effects be calculated.

#### ACKNOWLEDGMENT

The author is indebted to Professor Lichten for bringing the experimental results to his attention and for an instructive discussion of these results. It is also a pleasure to acknowledge a helpful correspondence with Dr. B. H. Bransden.

<sup>10</sup> K. Smith, Argonne National Laboratory Report ANL-6095, (unpublished).

<sup>11</sup> B. H. Bransden and J. S. C. McKee, Proc. Phys. Soc. (London) **A69**, 422 (1956).

<sup>12</sup> S. Gill, Proc. Cambridge Phil. Soc. **48**, 96 (1951).

<sup>13</sup> I. C. Percival and M. J. Seaton, Proc. Cambridge Phil. Soc. **53**, 654 (1957).