

Elastic scattering of electrons by hydrogen molecules

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Abstract. The differential and the total cross sections for the elastic scattering of 30–912 eV electrons by hydrogen molecules are calculated in the plane wave approximation. The interaction potential consists of the first order static potential and the second order adiabatic and non-adiabatic potentials. One-centre wavefunctions are employed to obtain the static potential and the effect of exchange is included by employing Ochkur approximation. The differential cross sections include terms up to only third order in the interaction energy and are in fair accord with the experimental data.

1. Introduction

Recently a number of theoretical investigations have been carried out for the scattering of electrons by the hydrogen molecule in which explicit allowance has been made for the polarization of the molecule. These investigations deal with the elastic scattering (Hara 1967, 1969a, Henry and Lane 1969) and with the rotational and vibrational excitations of the molecule (Lane and Geltman 1967, 1969, Lane and Henry 1968, Hara 1969b, Henry 1970). The polarization potentials are taken in the adiabatic approximation and are found to be of importance. However, all the above mentioned investigations are limited to low energy region (<10 eV). As a matter of fact the only recent theoretical investigation in the middle energy region is due to Khare and Moiseiwitsch (1965). These authors have employed first Born and first order exchange (Bell and Moiseiwitsch 1963) approximation. The polarization of the molecule has been completely ignored. A satisfactory agreement between their theoretical differential cross sections and the unnormalized data of Webb (1935) led them to believe that the polarization effects are not of importance. Recently William (1969) has measured the relative differential cross sections in the angular range 20° to 120° for 30–200 eV energy. Although the shape of his experimental curves are in good agreement with the theoretical curves of Khare and Moiseiwitsch for 100 and 200 eV impact energies, for 50 eV the difference between experiment and theory is quite evident for low scattering angles. This discrepancy may be attributed to the neglect of polarization effects. Further, even for higher impact energies polarization effects may be of importance for angles less than 20° .

To include the polarization effects Khare and Shobha (1970, 1971a, 1971b) have employed the plane wave approximation. In this approximation the electron is always represented by a plane wave but the adiabatic and the non-adiabatic distortions of the target atom are included in the form of local potentials. The contribution of exchange to the scattering amplitude is included by employing the Ochkur (1964) approximation.

The plane wave approximation has been successful in explaining the experimental differential cross sections for the elastic scattering of electrons by helium atoms. Hence, it seems of interest to adopt a similar procedure for investigating the elastic scattering of electrons by hydrogen molecules.

2. Theory

In the plane wave approximation the averaged differential cross section for the elastic scattering of the electron by an angle θ is given by (Khare and Shobha 1971a)

$$\overline{I(\theta)} = \overline{|(f_{B1} - g)|^2} + 2\overline{(f_{B1} - g)f_{dp}} \quad (1)$$

where f_{B1} and g are the first Born and the first order exchange scattering amplitudes, respectively. The second order scattering amplitude f_{dp} is given by†

$$f_{dp} = -\frac{1}{4\pi} \int \exp(i\mathbf{K} \cdot \mathbf{r}_1) V_{dp}(\mathbf{r}_1) d\mathbf{r}_1 \quad (2)$$

where \mathbf{K} is the change in the momentum vector of the incident electron due to scattering and \mathbf{r}_1 is the position vector of the incident electron referred to the centre of the molecule. $V_{dp}(\mathbf{r}_1)$ is the dynamic (adiabatic plus non-adiabatic) polarization potential. The bars denote the average over all orientations of the molecular axis. Equation (1) is correct to the third order in the interaction energy.

To evaluate f_{B1} and g we require a suitable wavefunction for the hydrogen molecule. Carter *et al* (1958) have given a spherically symmetric wavefunction and have employed it to obtain the phase shifts for the elastic scattering of low energy electrons. Their zero order phase shifts, are in good agreement with those calculated by Massey and Ridley (1956), using a two-centre wavefunction. The one-centre wavefunction of Carter *et al* is given by

$$\Psi(\mathbf{r}_2, \mathbf{r}_3) = \phi(\mathbf{r}_2)\phi(\mathbf{r}_3) \quad (3)$$

where \mathbf{r}_2 and \mathbf{r}_3 are the position vectors of the bound electrons referred to the centre of the molecule. The orbitals $\phi(\mathbf{r})$ can be represented with fair amount of accuracy by (Khare 1964)

$$\phi(\mathbf{r}) = \frac{N}{\pi^{1/2}} \{ \exp(-qr) + p(1+sr) \exp(-tqr) \} \quad (4)$$

with $N = 1.1895362$, $q = 1.0837$, $p = -0.4585$, $s = 1.196$ and $t = 4.1524$. For the interaction potential between the incident electron and the hydrogen molecule we have

$$V(\mathbf{r}_1; \mathbf{r}_2, \mathbf{r}_3) = -\frac{2}{r_{1A}} - \frac{2}{r_{1B}} + \frac{2}{r_{12}} + \frac{2}{r_{13}} \quad (5)$$

where the two nuclei are denoted by A and B. Using (3), (4) and (5) in the expression for f_{B1} and carrying out the elementary integration we obtain

$$f_{B1} = \frac{4}{K^2} \{ \cos(\frac{1}{2}\mathbf{K} \cdot \mathbf{R}) - J \} \quad (6)$$

† We use atomic units except for the energy which is expressed in Rydberg unless stated otherwise.

where \mathbf{R} denotes the vector formed by joining the two nuclei A and B and

$$J = 16N^2 \left(\frac{q}{(4q^2 + K^2)^2} + \frac{p(t+1)q}{\{(t+1)^2q^2 + K^2\}^2} + \frac{p^2tq}{\{4t^2q^2 + K^2\}^2} + \frac{ps\{3(t+1)^2q^2 - K^2\}}{\{(t+1)^2q^2 + K^2\}^3} \right. \\ \left. + \frac{sp^2(12t^2q^2 - K^2)}{(4t^2q^2 + K^2)^3} + \frac{12s^2p^2tq(4t^2q^2 - K^2)}{(4t^2q^2 + K^2)^4} \right). \quad (7)$$

In Ochkur approximation,

$$g = -\frac{2}{k_0^2} J \quad (8)$$

where k_0^2 is equal to the impact energy E_0 in Rydberg units. With (6), (8) and (1), $\overline{I}(\theta)$ is given in the first Born and Ochkur approximation ($f_{dp} = 0$) by

$$\overline{I}(\theta) = \frac{16}{K^4} \left\{ \frac{1}{2} \left(1 - \frac{\sin KR}{KR} \right) - 4J \left(1 - \frac{K^2}{2k_0^2} \right) \frac{\sin(\frac{1}{2}KR)}{KR} + J^2 \left(1 - \frac{K^2}{2k_0^2} \right)^2 \right\}. \quad (9)$$

It may be noted that Carter *et al* (1958) have taken the interaction potential as

$$V(r_1; r_2, r_3) = -v(r_1) + \frac{2}{r_{12}} + \frac{2}{r_{13}} \quad (10)$$

with

$$v(r_1) = \frac{8}{R} \quad \text{for } r_1 < \frac{1}{2}R \quad (11)$$

$$= \frac{4}{r_1} \quad \text{for } r_1 > \frac{1}{2}R. \quad (12)$$

Using (3) and (4) with (10) to (12) we get,

$$f_{B1} = \frac{4}{K^2} \left(\frac{\sin(\frac{1}{2}KR)}{\frac{1}{2}KR} - J \right). \quad (13)$$

It is easy to see that the first term of (13) oscillates about zero as K varies. Hence it produces oscillations in the differential cross sections for large values of K . These oscillations are not present in the experimental data and arise in the theory only because the interaction potential is given by (10). Hence, it may be concluded that the interaction potential employed by Carter *et al* for the calculations of the phase shifts is suitable only for low impact energies.

To examine the sensitivity of $\overline{I}(\theta)$ for the ground state wavefunction we have employed another one centre wavefunction given by Huzinaga (1957). This wavefunction has been extensively utilized by Khare in investigating the excitation of the hydrogen molecule to six low lying singlet and triplet states (Khare 1966a, 1966b, 1967) and also to obtain photo-ionization cross sections (Khare 1968). Practically in all cases satisfactory results are obtained. The wavefunction of Huzinaga is given by

$$\psi(r_2, r_3) = \frac{c_1}{2^{1/2}} (\phi_{in}(r_2)\phi_{out}(r_3) + \phi_{out}(r_2)\phi_{in}(r_3)) + c_2\phi_{lr}(r_2)\phi_{lr}(r_3) \quad (14)$$

where

$$\phi_{\text{in}}(r) = c_3 \{N(1, \xi_1) \exp(-\xi_1 r) Y_{00} + (\delta Y_{00} + \lambda Y_{20}) N(4, \xi_2) r^3 \exp(-\xi_2 r)\} \quad (15)$$

$$\phi_{\text{ir}}(r) = N(2, z) r \exp(-zr) Y_{10} \quad (16)$$

$$\phi_{\text{out}}(r) = N(1, \eta_1) \exp(-\eta_1 r) Y_{00} \quad (17)$$

$$N(n, \chi) = \frac{(2\chi)^{n+1/2}}{\{(2n)!\}^{1/2}} \quad (18)$$

and Y_{lm} are normalized spherical harmonics. The value of the various parameters occurring in (14) to (17) are given by Khare (1966a) and need not be repeated here. Using the above wavefunction in the first Born and Ochkur approximation we get

$$\begin{aligned} \overline{I(\theta)} = \frac{16}{K^4} \left\{ \frac{1}{2} \left(1 + \frac{\sin KR}{KR} \right) - \left(1 - \frac{K^2}{2k_0^2} \right) \{ 2A j_0(\tfrac{1}{2}KR) - 2\sqrt{(5)} B j_2(\tfrac{1}{2}KR) + 6C j_4(\tfrac{1}{2}KR) \} \right. \\ \left. + \left(1 - \frac{K^2}{2k_0^2} \right)^2 (A^2 + B^2 + C^2) \right\}. \end{aligned} \quad (19)$$

where $j_l(x)$ are the spherical Bessel functions. The expressions for A , B and C are as follows:

$$\begin{aligned} A = \frac{c_1^2 c_3^2}{2} \left\{ N^2(1, \xi_1) J(0, \xi_1, \xi_1, 2) + (\delta^2 + \lambda^2) N^2(4, \xi_2) \right. \\ \times J(0, \xi_2, \xi_2, 8) + 2\delta N(1, \xi_1) N(4, \xi_2) J(0, \xi_1, \xi_2, 5) \\ + 2N^2(1, \eta_1) \left(N(1, \xi_1) \frac{2!}{(\eta_1 + \xi_1)^3} + \frac{5! \delta N(4, \xi_2)}{(\eta_1 + \xi_2)^6} \right) \\ \times \{ N(1, \xi_1) J(0, \xi_1, \eta_1, 2) + \delta N(4, \xi_2) J(0, \xi_2, \eta_1, 5) \} \\ + N^2(1, \eta_1) J(0, \eta_1, \eta_1, 2) \left(1 + \delta^2 + \lambda^2 + \frac{2\delta N(1, \xi_1) N(4, \xi_2) 5!}{(\xi_1 + \xi_2)^6} \right) \\ \left. + c_2^2 N^2(2, z) J(0, z, z, 4) \right\} \end{aligned} \quad (20)$$

$$\begin{aligned} B = -c_1^2 c_3^2 \left\{ \lambda N(1, \xi_1) N(4, \xi_2) J(2, \xi_1, \xi_2, 5) + \lambda(\delta + \tfrac{1}{2}\lambda\sqrt{5}) N^2(4, \xi_2) J(2, \xi_2, \xi_2, 8) \right. \\ + \lambda N^2(1, \eta_1) N(4, \xi_2) \left(\frac{2! N(1, \xi_1)}{(\xi_1 + \eta_1)^3} + \frac{5! \delta N(4, \xi_2)}{(\xi_2 + \eta_1)^6} \right) J(2, \xi_2, \eta_1, 5) \Big\} \\ - \frac{2}{\sqrt{5}} c_2^2 N^2(2, z) J(2, z, z, 4) \end{aligned} \quad (21)$$

and

$$C = \tfrac{3}{2} c_1^2 c_3^2 \lambda^2 N^2(4, \xi_2) J(4, \xi_2, \xi_2, 8) \quad (22)$$

where

$$J(l, p, q, s) = \int j_l(Kr) \exp\{-(p+q)r\} r^s dr. \quad (23)$$

Another calculation in the first Born and the first order exchange approximation carried out by Khare and Moiseiwitsch (1965) employing a two-centre wavefunction is also available for comparison.

To calculate f_{dp} we need the dynamic polarization potential $V_{dp}(r_1)$. We have carried out a multipole expansion of the potential and have retained only those terms which do not fall asymptotically faster than r_1^{-6} . Thus

$$V_{dp}(r_1) = V_p^1(r_1) + V_p^2(r_1) + V_d^1(r_1) \quad (24)$$

where $V_p^l(r_1)$ and $V_d^l(r_1)$ are the l th multipole components of the adiabatic and non-adiabatic potentials respectively (Khare and Shobha 1971a). Following Hara (1967) we take

$$V_p^1(r_1) = -\frac{\alpha_d}{(r_1^2 + R_0^2)^2} - \frac{\alpha'_d r_1^2 P_2(\cos \theta_1)}{(r_1^2 + R_0^2)^3} \quad (25)$$

where $P_l(\cos \theta)$ are the Legendre polynomials and R_0 is a cut-off parameter and has been taken equal to 1.6 (Hara 1967). α_d , the mean dipole polarizability, and α'_d , a measure of the anisotropy of the polarizability, are given by

$$\alpha_d = \frac{1}{3}(\alpha_z + 2\alpha_x) \quad (26)$$

and

$$\alpha'_d = \frac{2}{3}(\alpha_z - \alpha_x). \quad (27)$$

α_z and α_x are the dipole polarizabilities of the hydrogen molecule along the internuclear axis and perpendicular to the axis, respectively. Using the values of Kolos and Wolniewicz (1967) for α_z and α_x we get $\alpha_d = 5.18$ and $\alpha'_d = 1.20$.

Expressions are not available for $V_p^2(r_1)$ and $V_d^1(r_1)$. $V_p^2(r_1)$ falls asymptotically as $-\alpha_q/r_1^6$ where α_q is the mean quadrupole polarizability of the molecule. Due to finite velocity of the incident electron the polarization potential does not remain $V_p^1(r_1) + V_p^2(r_1)$ but becomes less attractive by an amount equal to $V_d^1(r_1)$. For slow moving electron $V_d^1(r_1)$ falls asymptotically as $6\beta_1/r_1^6$ (see Dalgarno *et al* 1968 for the definition of β_1). Hence we have taken

$$V_p^2(r_1) + V_d^1(r_1) = \frac{(6\beta_1 - \alpha_q)r_1^2}{(r_1^2 + R_0^2)^4}. \quad (28)$$

The behaviour of the above potentials for small values of r_1 is chosen in a rather arbitrary way. The values of β_{1z} and β_{1x} are available (Dalgarno *et al* 1968). Using those values and a formula similar to (26) we get $\beta_1 = 5.03$. For α_q no theoretical or experimental value seems to be available. Recognizing that two hydrogen atoms are the separated atom limit of H_2 we calculate α_q by the following simple scaling relation

$$\left(\frac{\alpha_q}{\alpha_d}\right)_{H_2} = \left(\frac{\alpha_q}{\alpha_d}\right)_H. \quad (29)$$

This has yielded a value of 17.27 for α_q . It may be noted that if we replace α_q by β_1 in (29) we get β_1 for H_2 equal to 6.19 which is close to the value of β_1 derived above. This may give some justification for the use of (29). Since helium is the united atom limit of the hydrogen molecule we have also employed (29) after replacing H by He in the right hand side and obtained α_q and β_1 equal to 8.64 and 2.63 respectively. This value of β_1 is not in agreement with the previously derived value of 5.03. Hence it may be expected that α_q equal to 17.27 is more appropriate and we have used this value of α_q unless specified otherwise.

It may also be noted that $\psi(r_2, r_3)$ as given by (3) and (4) is spherically symmetric. Hence the static potential of the molecule will be asymptotically of the form

$$V_{00}(r_1) \underset{r_1 \rightarrow \infty}{\sim} -\frac{4(\frac{1}{2}R)^2}{r_1^3} P_2(\cos \theta_1) + O(r_1^{-5}). \quad (30)$$

However the leading term should have been $-(2Q/r_1^3)P_2(\cos \theta_1)$, where Q is the quadrupole moment of the molecule. To correct for this discrepancy we have added another potential $V_Q(r_1)$ given by

$$V_Q(r_1) = \frac{2(\frac{1}{2}R^2 - Q)}{(r_1^2 + R_0^2)^3} r_1^3 P_2(\cos \theta_1). \quad (31)$$

Equation (31) is similar to the potential taken by Hara (1967). The value of Q equal to 0.484 (Kolos and Wolniewicz 1967) is taken and $V_{dp}(r_1)$ in (2) is replaced by the sum of (25), (28) and (31) (to be referred as V_I). $I(\theta)$ are then calculated with the help of (1), (2), (6), (7) and (8) for energy varying from 30 eV to 912 eV. Finally $I(\theta)$ are integrated to obtain total cross section. To bring out the importance of the long range potentials which fall asymptotically as r_1^{-6} another set of differential and total cross sections are obtained with $\alpha_q = \beta_1 = 0$.

To examine the sensitivity of the cross sections for the long range potentials we have used another adiabatic dipole polarization potential given by (Henry and Lane 1969).

$$V_p^1(r_1) = v_0^1(r_1) + v_2^1(r_1) P_2(\cos \theta_1) \quad (32)$$

where

$$v_0^1(r_1) = -\frac{\alpha_d}{(r_1^2 + r_c^2)^2} \left[1 - \exp \left\{ -\left(\frac{r_1}{r_a} \right)^3 \right\} \right] \quad (33)$$

and

$$v_2^1(r_1) = -\frac{\alpha'_d}{(r_1^2 - r_d^2)^2} \left[1 - \exp \left\{ -\left(\frac{r_1}{r_b} \right)^4 \right\} \right] \quad \text{for } r_1 \geq 0.5 \quad (34)$$

$$= 0 \quad \text{for } r_1 < 0.5. \quad (35)$$

For $V_Q(r_1)$ we take

$$V_Q(r_1) = \frac{2(\frac{1}{2}R^2 - Q)}{r_1^3} \left[1 - \exp \left\{ -\left(\frac{r_1}{r_e} \right)^6 \right\} \right] \quad (36)$$

which is a modified form of the potential employed by Henry and Lane (1969). The values of the parameters r_a , r_b , r_c , r_d and r_e , as given by the above mentioned authors are, 1.7, 2.0, 1.22, 0.1 and 1.8, respectively. Consistent with (33) and its own asymptotic behaviour we have taken

$$V_p^2(r_1) + V_d^1(r_1) = \frac{(6\beta_1 - \alpha_q)}{(r_1 + r_c)^3} \left[1 - \exp \left\{ -\left(\frac{r_1}{r_a} \right)^3 \right\} \right]. \quad (37)$$

After replacing $V_{dp}(r_1)$ by the sum of (32), (36) and (37) (to be referred as V_{II}) the cross sections are again calculated. Finally in (37) we take $\alpha_q = 8.64$ and using V_{II} another set of cross sections are obtained.

3. Results and discussions

The differential cross sections obtained from (9) without and with exchange are shown in figure 1 by the curves A and B respectively. The later cross sections are denoted by \bar{I}_B and those obtained from (19) are denoted by \bar{I}_D .

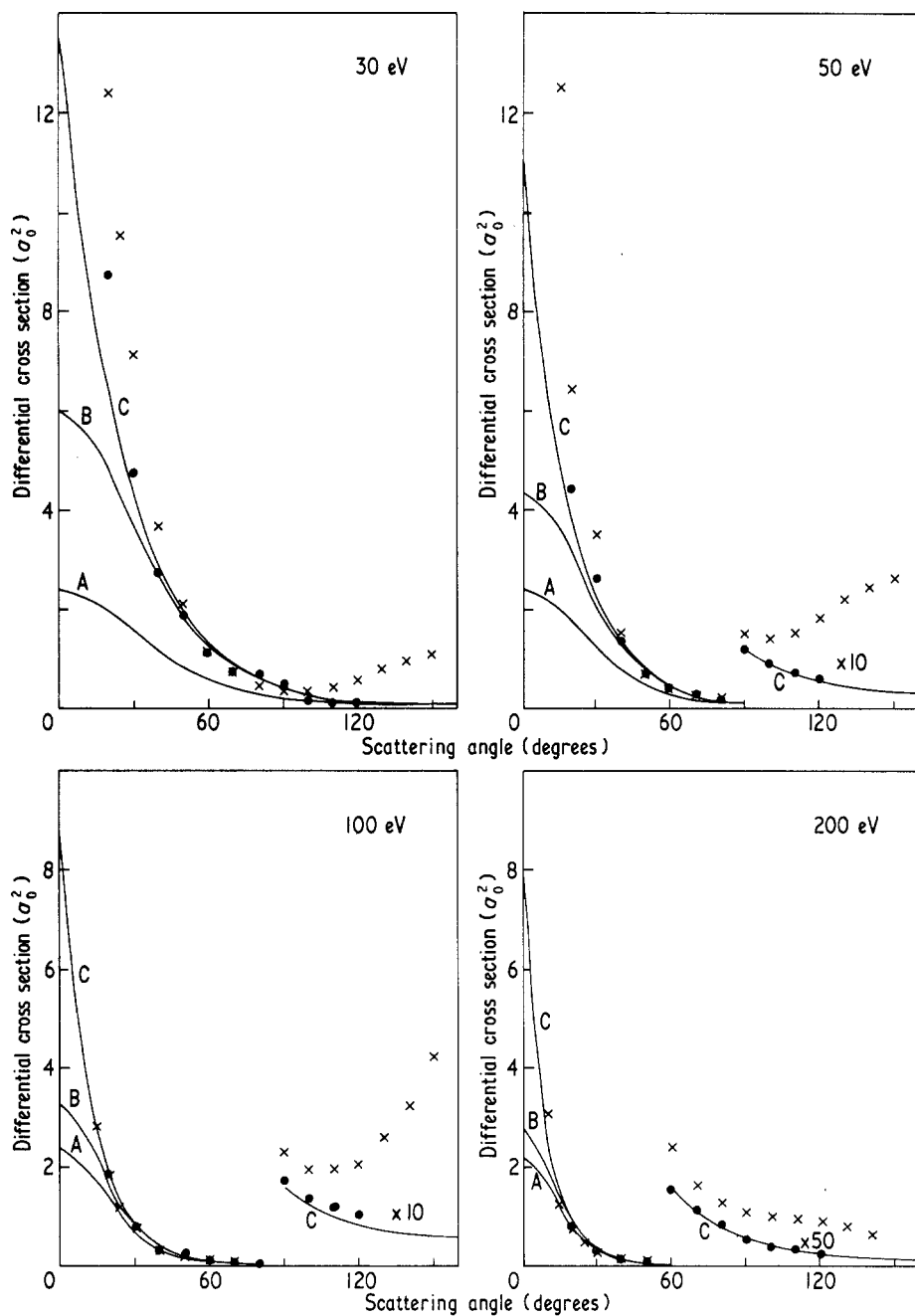
In all the calculations which include long range potentials the molecule is always represented by (3) and (4). However as pointed out earlier f_{dp} are calculated with the following different expressions for $V_{dp}(r_1)$:

- (i) $V_{dp}(r_1) = V_I$ (the sum of (25), (28) and (31))
- (ii) $V_{dp}(r_1) = V_I$ as in (i) but with $\alpha_q = \beta_1 = 0$
- (iii) $V_{dp}(r_1) = V_{II}$ (the sum of (32), (36) and (37))
- (iv) $V_{dp}(r_1) = V_{II}$ as in (iii) but with $\alpha_q = 8.37$.

The differential cross sections $\bar{I}(\theta)$ obtained from (1) for the cases (i), (ii), (iii) and (iv) are denoted by \bar{I}_C , \bar{I}_E , \bar{I}_F and \bar{I}_G , respectively.

Let us now consider figure 1. It compares the present theoretical results with the experimental data of Webb (1935) and of William (1969). As the data are unnormalized, for comparison we have adopted the procedure employed by William. Both laboratory measurements have been scaled for their best visual fit to the theoretical curves C for the angular range over which they have the same general shape. Starting from the highest impact energy (912 eV) we find that the effect of exchange is negligible (curves A are not shown for 350 eV, 600 eV and 912 eV for the sake of clarity) and the effect of polarization is limited to very low angle ($<10^\circ$). The agreement between the theory and the experiment is satisfactory for the whole angular range. For 600 eV and 350 eV impact energies we note that the inclusion of the polarization effects has improved the agreement between the theory and the experiment. However, for 350 eV impact energy the experimental data (Webb 1935) lie above the theoretical curve for large angles. Such a behaviour of the experimental data of Webb (1935) continues also to the lower impact energies and is markedly different from that obtained by William (1969). For the lower impact energies it is evident from the figure that the inclusion of exchange and polarization has considerably improved the agreement between the theory and the experiment. Even for an energy as low as 30 eV the plane wave approximation yields differential cross sections which are in fair accord with the recent experimental data. This seems better than expected. It may be noted that our theoretical curves are in much better agreement with the data of William (1969) than with those of Webb (1935). However, the data of William do not cover the angles smaller than 20° where the polarization effects are found to be of importance.

In table 1 we have compared the values of $\bar{I}(\theta)$ obtained from (1) with $f_{dp} = 0$. The hydrogen molecule is represented by three different wavefunctions. The second to fourth columns show that for the small values of K the differential cross sections obtained from (19) are higher than those obtained by the use of (9). The ratios are practically unity for the large values of K but for the medium values of K the ratios are less than unity. While examining the next three columns it may be noted that Khare and Moiseiwitsch have employed a two-centre wavefunction and the exchange scattering amplitude is obtained in the separated atom limit by employing first order exchange approximation (Bell and Moiseiwitsch 1963). However, at 912 eV the effect of exchange is negligible and at 200 eV the two exchange approximations (first order exchange and Ochkur) are expected to yield same exchange scattering amplitude. Hence the last two columns of table 1 mainly compare the effects of two different wavefunctions. The



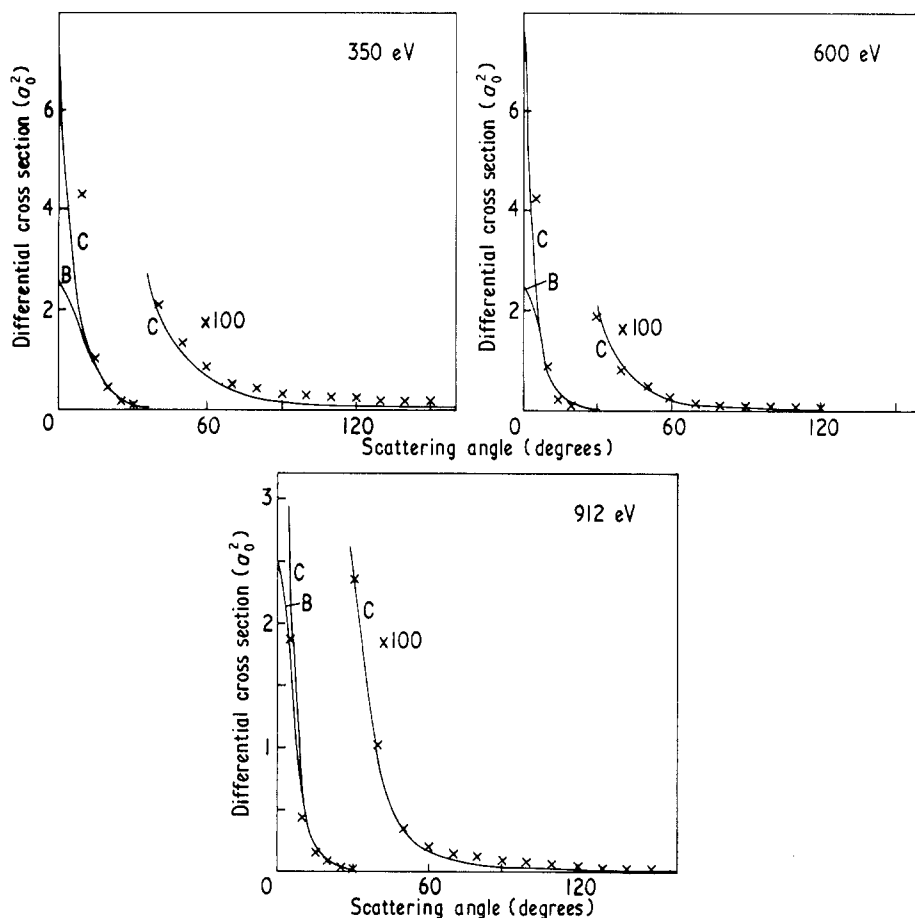


Figure 1. Curve A, first Born approximation; curve B, first Born and Ochkur approximation; curve C, plane wave approximation. The long range potential is the sum of (25), (28) and (31) (referred to as V_l , see text). ● and × are the experimental data of William (1969) and Webb (1935) respectively. The energy of the incident electron E_0 is indicated in the figure and '× 10' etc. represents the multiplication factors.

ratios are less than unity for the small values of K and are approximately unity for the large values of K . The three wavefunctions which are employed to calculate the differential cross sections are quite different from one another. However the ratios do not differ from unity by more than about 20%. In table 2 the results obtained by the use of different long range potentials are compared. The second to fourth columns show that the effect of ignoring the potentials which fall asymptotically as r_1^{-6} is to increase the cross sections for the low angles. However the increase is within 20% and is almost independent of the impact energy. The next three columns compare the differential cross sections obtained with long range potentials V_{II} and V_I . In general for the small values of K , the potential V_{II} yields higher cross sections but the ratios become less than unity with the increase of K . Although the two potentials are significantly different from one another for small values of r_1 , the ratios do not differ from unity by more than 15%. The next three columns show that the decrease in the value of α_q results in

Table 1.†

$\cos \theta$	E_0 (eV)	I_D/I_B			I_{KM}/I_B		
		50	200	912	50	200	912
1.00		1.18	1.22	1.24	0.93	0.85	0.82
0.99		1.16	1.15	1.01	0.87	0.88	—
0.98		1.15	1.10	0.94	0.86	0.90	0.84
0.97		1.13	1.05	0.91	0.87	0.84	0.87
0.95		1.11	1.00	0.90	0.88	0.91	—
0.90		1.06	0.93	0.92	0.90	0.83	1.03
0.80		1.00	0.92	0.97	0.94	0.82	0.92
0.70		0.98	0.93	0.99	0.97	0.91	1.04
0.60		0.97	0.94	1.00	0.97	0.93	0.99
0.40		1.03	0.97	1.00	1.01	0.94	0.92
0.20		1.02	0.99	1.00	0.98	0.99	0.98
0.00		1.00	1.00	1.00	0.99	1.02	1.02
−0.20		1.02	1.00	1.00	0.97	1.03	0.99
−0.40		1.04	1.01	1.00	0.91	1.06	0.97
−0.60		1.06	1.01	1.00	0.99	1.06	0.96
−0.80		1.07	1.00	1.00	1.02	1.03	1.01
−1.00		1.08	1.00	1.00	1.04	0.05	1.03

† The differential cross sections I_{KM} are obtained from Khare and Moiseiwitsch.

Table 2.

$\cos \theta$	E_0 (eV)	I_E/I_C			I_F/I_C			I_G/I_F		
		30	200	912	30	200	912	30	200	912
1.00		1.11	1.13	1.13	1.10	1.12	1.12	0.88	0.86	0.86
0.99		1.13	1.19	1.15	1.13	1.14	0.97	0.85	0.78	0.78
0.98		1.14	1.18	1.08	1.13	1.08	0.88	0.84	0.77	0.88
0.97		1.14	1.17	1.03	1.13	1.04	0.87	0.83	0.77	0.97
0.95		1.14	1.14	0.99	1.11	0.96	0.96	0.83	0.80	1.05
0.90		1.14	1.07	0.99	1.09	0.87	1.10	0.82	0.90	1.02
0.80		1.12	1.00	1.00	1.03	0.93	0.97	0.83	1.04	0.99
0.70		1.11	0.98	1.00	0.99	1.04	1.06	0.85	1.05	1.03
0.60		1.09	0.98	1.00	0.96	1.01	0.99	0.87	1.03	1.07
0.40		1.06	1.00	1.00	0.92	1.07	1.03	0.92	1.01	1.00
0.20		1.04	1.00	1.00	0.90	0.99	0.96	0.96	0.99	0.99
0.00		1.02	1.00	0.99	0.91	0.97	1.01	1.00	0.99	0.97

the decrease of differential cross sections. However, the ratio I_G/I_F is not less than 0.77 although the two values of α_q differ from one another by about a factor of two. We may conclude from the tables 1 and 2 that the cross sections are not very sensitive to the wavefunction and to the detailed nature of the long range potential for the small values of r_1 .

Table 3 shows that the difference between the total cross sections with and without exchange is large for the low impact energies and it decreases with the increase of energy. Further we find that the use of Huzinaga's wavefunction yields higher cross sections

Table 3.

E_0 (eV)	Total cross sections (a_0^2)						
	Q_A^\dagger	Q_B^\ddagger	Q_C	Q_D	Q_E	Q_F	Q_G
30	5.99	13.1	15.0	13.7	16.5	15.3	13.3
50	3.82	6.20	7.15	6.44	7.93	7.33	6.30
100	2.03	2.58	2.99	2.66	3.33	3.07	2.62
200	1.04	1.18	1.37	1.20	1.53	1.41	1.20
350	0.60	0.65	0.75	0.66	0.84	0.78	0.66
600	0.35	0.37	0.44	0.37	0.49	0.45	0.38
912	0.23	0.24	0.29	0.25	0.32	0.30	0.25

$^\dagger Q_A$ are the total cross sections in the first Born approximation, the molecule being represented by (3) and (4).

$^\ddagger Q_B, Q_C, Q_D, Q_E, Q_F$, and Q_G are obtained by integrating the differential cross sections represented by I_B, I_C, I_D, I_E, I_F , and I_G respectively.

in comparison of those obtained by employing (3) and (4). However, the difference is within a few percent. The change in the total cross sections by the inclusion of the long range potential is much less in comparison to the change produced by it in the differential cross sections. We also note that the cross sections Q_E and Q_F are greater than Q_C and Q_G , respectively. All these observations are consistent with tables 1 and 2. No other theoretical or experimental results for the total cross sections are available. However, Carter *et al* (1958) obtained $\sum_{l=0}^{\infty} Q_l$ equal to 6.15 in the static field approximation for $k_0 = 1.3$. This value is consistent with the present first Born value of 5.99 for $E_0 = 30$ eV.

It may be noted that we have employed a potential $V_d^1(r_1)$ to correct the adiabatic potential. This correction is expected to be of right magnitude only for slow moving electrons. Hence the polarization effects produced by V_I and V_{II} may not be correct for higher impact energies. However, an examination of the curves C of figure 1 shows that for higher impact energies the effect of polarization is limited to small angles. At these angles a large number of partial waves contribute. For higher partial waves the correction obtained by $V_d^1(r_1)$ is expected to be of right magnitude. Furthermore, in the investigation of the elastic scattering of electrons by the helium atoms it was found (Khare and Moiseiwitsch 1965) that the fractional increase in the low order phase shifts from their static field values due to the effect of polarization potential is small at high energies. The same behaviour may be expected for the hydrogen molecule also.

Finally we may conclude that although many simplifying assumptions have been employed, the above discussions indicate that more accurate theoretical cross sections may not be widely different from those presented by curves C of figure 1 and Q_C . It is certainly desirable that absolute values of the cross sections over wide angular and energy ranges be made available for comparison.

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