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e^-–H_2 elastic scattering over 100–1000 eV

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Abstract. A method proposed by Das has been employed to calculate the elastic differential cross section and the total collisional cross section for the electrons scattered by the hydrogen molecule. The total collisional cross sections and the real part of the forward elastic scattering amplitudes are also obtained for the scattering of electrons by H and He atoms. The theoretical results are compared with the available experimental and other accurate theoretical data. We have found that the present results for the differential cross section are in reasonable agreement only at the intermediate angles.

1. Introduction

Recently Das (1978) has suggested a simple method (to be referred to hereafter, as the Das method) to compute differential cross sections (DCS) for the scattering of electrons by a potential. Later on the method was extended to the elastic scattering of electrons (e^-) and positrons (e^+) by H and He atoms (Das and Biswas 1980, 1981, Das *et al* 1981, Das and Saha 1981). Reasonable agreement between theory and the experiments for the above systems has been obtained by Das and his associates. However, they have computed only DCS for the elastic scattering of electrons by hydrogen and helium atoms. It is also of interest to calculate forward scattering amplitudes and compare the real part with the dispersion relation results and the imaginary part with the theoretical and experimental total collisional cross sections, by using the optical theorem. Similarly the total elastic cross sections may also be obtained and compared with the available theoretical and experimental data. Further, the Das method has not been applied so far to any molecular target. Just as the hydrogen atom provides the simplest atomic target, the hydrogen molecule is the simplest molecular target which may be employed to test the validity of any new method. Reliable and absolute experimental data for the elastic DCS (van Wingerden *et al* 1977, Fink *et al* 1975, Lloyd *et al* 1974) as well as the total collision cross sections (Dalba *et al* 1980, van Wingerden *et al* 1980, Hoffman *et al* 1982) along with a good number of successful theoretical investigations (Jhanwar *et al* 1982b and the references given therein) are available in the intermediate energy range for e^-–H_2 scattering to assess the accuracy of a new theoretical model. Hence it is of interest to extend the application of the Das method to e^-–H_2 elastic scattering. In the present investigation we have covered the 100–1000 eV energy range.

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2. Theory

The scattering amplitude in the Das method, f^{out} or f_{Das}, is obtained by solving the relevant Fredholm integral equation with the help of a trial amplitude f_t (Das 1978). The trial amplitude f_t is taken to be of the form $(a(E)+ib(E))f_{B1}$, f_{B1} being the amplitude in the first Born approximation. The variational energy dependent and real parameters a and b are determined by minimising the values of

$$\int |f^{\text{out}}-f_t|^2 \sin\theta \, d\theta$$

where θ is the scattering angle. Thus, one finally obtains (Das *et al* 1981)

$$f^{\text{out}}=f_{\text{Das}}=f_{B1}+a \operatorname{Re} f_{B2}-b \operatorname{Im} f_{B2}+i(a \operatorname{Im} f_{B2}+b \operatorname{Re} f_{B2}) \tag{1}$$

with a and b given by

$$a=\frac{\int d\theta \sin\theta f_{B1}(f_{B1}-\operatorname{Re} f_{B2})}{\int d\theta \sin\theta[(f_{B1}-\operatorname{Re} f_{B2})^2+(\operatorname{Im} f_{B2})^2]} \tag{2}$$

$$b=\frac{\int d\theta \sin\theta f_{B1} \operatorname{Im} f_{B2}}{\int d\theta \sin\theta[(f_{B1}-\operatorname{Re} f_{B2})^2+(\operatorname{Im} f_{B2})^2]}. \tag{3}$$

In the above equations $\operatorname{Re} f_{B2}$ and $\operatorname{Im} f_{B2}$ represent the real and the imaginary parts of the second Born amplitude, respectively.

It may be noted that in the Das method the direct DCS is given by

$$I_{\text{Das}}=|f_{\text{DAS}}|^2=|f_{B1}|^2+|f_{B2}|^2(a^2+b^2)+2f_{B1}(a \operatorname{Re} f_{B2}-b \operatorname{Im} f_{B2}). \tag{4}$$

The differential cross section in the second Born approximation (I_{B2}) is also given by (4) but with $a=1$ and $b=0$. It is then easy to see that

$$I_{B2}-I_{\text{Das}}=|f_{B2}|^2(1-a^2-b^2)+2f_{B1}[(1-a) \operatorname{Re} f_{B2}+b \operatorname{Im} f_{B2}]. \tag{5}$$

For hydrogen and helium atoms, the variational parameters a and b are positive and in general less than unity (see table 3 of Das and Saha 1981) such that as the energy increases a increases and b decreases towards their limiting values of unity and zero, respectively. Thus, in general, $I_{\text{Das}}<I_{B2}$.

The extension of the theory for the case of e^-–H_2 elastic scattering needs only a little modification. The scattering amplitudes now depend on the orientation of the molecular axis, denoted by $\boldsymbol{R}=(R, \theta_R, \phi_R)$, $2R$ being the internuclear distance. The results, therefore, are to be averaged over all molecular orientations. The Das scattering amplitude is still given by the same expression (1) but now $a(H_2)$ and $b(H_2)$ are to be determined by minimising the values of

$$\int d\Omega_R \int d\theta \sin\theta |f^{\text{out}}-f_t|^2$$

where Ω_R denotes the molecular orientation of the molecular axis. Thus (2) and (3) modify to

$$a(H_2)=\frac{\int d\Omega_R \int d\theta \sin\theta f_{B1}(f_{B1}-\operatorname{Re} f_{B2})}{\int d\Omega_R \int d\theta \sin\theta[(f_{B1}-\operatorname{Re} f_{B2})^2+(\operatorname{Im} f_{B2})^2]} \tag{6}$$

and

$$b(H_2) = \frac{\int d\Omega_R \int d\theta \sin\theta f_{B1} \operatorname{Im} f_{B2}}{\int d\Omega_R \int d\theta \sin\theta [(f_{B1} - \operatorname{Re} f_{B2})^2 + (\operatorname{Im} f_{B2})^2]}. \tag{7}$$

The averaged DCS, including exchange, is then obtained by

$$I(H_2) = \frac{1}{4\pi} \int d\Omega_R |f - g_{GO}|^2 \tag{8}$$

where g_{GO} is the Glauber–Ochkur exchange amplitude for e^-–H_2 elastic scattering.

Quite recently Jhanwar *et al* (1982b) have employed two-centre Weinbaum-type wavefunctions (Weinbaum 1933) to compute f_{B1} and f_{B2} in their calculation of e^-–H_2 elastic scattering in the modified Glauber approximation. They obtained fairly good agreement with the experimental data (see tables 1 and 2) thus indicating the suitability of the wavefunction. Weinbaum's wavefunction is a two-parameter variational wavefunction having partial ionic character. The value of the dissociation energy obtained by the above wavefunction is 4.00 eV which is better than those given by extreme atomic orbitals (Wang's wavefunction) and molecular orbital (LCAO–MO) treatments. The value of R as given by Weinbaum's wavefunction is also only 4% different from the experimental data (see Pauling and Wilson 1935 for the references and the discussion). It may also be noted that Gupta and Khare (1978), who compared the first Born DCS obtained by the highly accurate one-centre wavefunction of Hayes (1967), the highly accurate two-centre wavefunctions employed by Ford and Browne (1973) and Liu and Smith (1973) and the one-centre wavefunction of Joy and Parr (1958), observed that the cross sections are not very sensitive to the wavefunction. Following Jhanwar *et al* (1982b) in the present investigation we have also employed two-centre Weinbaum-type wavefunctions. In order to make the calculation tractable Jhanwar *et al* employed the separated-atom approximation i.e. the two-centre integrals were neglected. They also took

$$\int \cos(\overline{\boldsymbol{q} - \boldsymbol{k}_f} \cdot \boldsymbol{R}) \cos(\overline{\boldsymbol{k}_i - \boldsymbol{q}} \cdot \boldsymbol{R}) T(\boldsymbol{q}, \boldsymbol{k}_i, \boldsymbol{k}_f)\, d\boldsymbol{q} = \cos(\boldsymbol{K} \cdot \boldsymbol{R}) \int T(\boldsymbol{q}, \boldsymbol{k}_i, \boldsymbol{k}_f)\, d\boldsymbol{q} \tag{9}$$

under the condition that $T(\boldsymbol{q}, \boldsymbol{k}_i, \boldsymbol{k}_f)$ is a slowly varying function of $\boldsymbol{q}$. In (9) $\boldsymbol{k}_i$ and $\boldsymbol{k}_f$ are the initial and final momentum vectors of the incident electron and $\boldsymbol{K}(=\boldsymbol{k}_i - \boldsymbol{k}_f)$ is the momentum transfer vector during the collision. Using the above approximation they obtained a cute relationship given by

$$f_{Bn}(H_2) = \cos(\boldsymbol{K} \cdot \boldsymbol{R}) f_{Bn}(He) \qquad \text{for } n = 1 \text{ and } 2 \tag{10}$$

where $f_{Bn}(He)$ is the nth Born scattering amplitude for the helium atom represented by

$$\psi_{He}(\boldsymbol{r}_1, \boldsymbol{r}_2) = (Z^3/\pi) \exp[-Z(\boldsymbol{r}_1 + \boldsymbol{r}_2)]. \tag{11}$$

with $Z = 1.2005$, a value appropriate for the hydrogen molecular Weinbaum wavefunction for $R = 0.7$. Using (10) in (6) and (7) we notice that a and b become similar to those given by (2) and (3), respectively, with a weight factor of $(J_0(KR) + 1)$, where f_{B1} and f_{B2} are now appropriate to the helium atom represented by (11). Following Jhanwar *et al* (1982b) it is assumed that $g_{GO}(H_2)$ and $g_{GO}(He)$ are also related by (10) and then the averaged DCS for H_2 is obtained by (8).

Let us now compare the Das method with the modified Glauber approximation (MG) which has been successfully utilised by Jhanwar *et al* (1982b) for e^-–H_2 elastic

scattering. The scattering amplitude in MG is given by

$$f_{MG} = f_G - f_{G2} + f_{B2} \tag{12}$$

where f_{G2}, which is purely imaginary, is the second term of the Glauber series obtained by expanding the Glauber amplitude f_G in the powers of interaction potential. If we also write f_{MG} in the form given by (1) with the help of the coefficients a_{MG} and b_{MG} then it is easy to see that

$$a_{MG} = 1 + \frac{\mathrm{Re}\,(f_G - f_{B1})\,\mathrm{Re}\,f_{B2} + \mathrm{Im}(f_G - f_{G2})\,\mathrm{Im}\,f_{B2}}{|f_{B2}|^2} \tag{13}$$

$$b_{MG} = \frac{\mathrm{Im}(f_G - f_{G2})\ \mathrm{Re}\,f_{B2} - \mathrm{Re}(f_G - f_{B1})\,\mathrm{Im}\,f_{B2}}{|f_{B2}|^2}. \tag{14}$$

Since f_{B1}, f_{B2}, f_G and f_{G2} are all dependent on the molecular orientation as well as on the angle of scattering, the coefficients a_{MG} and b_{MG} are functions of incident energy, scattering angle and molecular orientation. However, using (10) we find that a_{MG} and b_{MG} no longer depend upon the molecular orientation but, unlike Das parameters, they are still functions of the scattering angle.

Finally, we have integrated expression (8) over the scattering angles to obtain the total elastic cross section. The total collisional cross sections are also obtained from the imaginary part of the forward scattering amplitude with the help of the optical theorem. We have also used the Das method to obtain the real and imaginary parts of the forward scattering amplitude for e^-–H and e^-–He elastic scattering. The amplitudes f_{B1} and f_{B2} for these targets are obtained in a manner identical to that employed by Jhanwar *et al* (1982a).

3. Results and discussion

In figure 1 a_{Das} and b_{Das} are compared with a_{MG} and b_{MG} for the hydrogen molecule at impact energies 100, 200, 400 and 1000 eV. As expected a_{Das} and b_{Das}, which are independent of the scattering angle, move towards their asymptotic values ($a = 1$ and $b = 0$) as the energy increases. a_{MG} and b_{MG} vary with scattering angles and the range of variation in a_{MG} decreases with the increase of the incident energy. However, the values of b_{MG} increase as the energy changes from 100 to 200 eV. A further increase of the incident energy results in decreasing values for b_{MG}. The figure further shows that at small angles $a_{MG} > a_{Das}$ while at large angles the reverse is the case. On the other hand at 100 and 200 eV b_{Das} is always greater than b_{MG} but at 400 and 1000 eV b_{MG} overtakes b_{Das} at some intermediate angles. From figure 1 and the relation (1) it is expected that I_{Das} will be less than I_{MG} at small angles and greater than I_{MG} at large angles. This expectation finds support from the values listed in table 1. In this table we have shown the ratios I_{Das}/I_{expt} and I_{MG}/I_{expt} as functions of the scattering angle. The table shows that the difference between I_{Das} and I_{MG} for small angles decreases as the incident energy increases. However, the differences at large angles are practically independent of the incident energy. For example, at 130° I_{Das} is about 1.5 times I_{MG} at all the four energies under consideration.

Now a comparison of I_{Das} with I_{expt} clearly shows that at 100 eV the Das method greatly underestimates the DCS at small angles and the underestimate decreases with the increase of angle resulting in a better agreement at larger angles. On the other

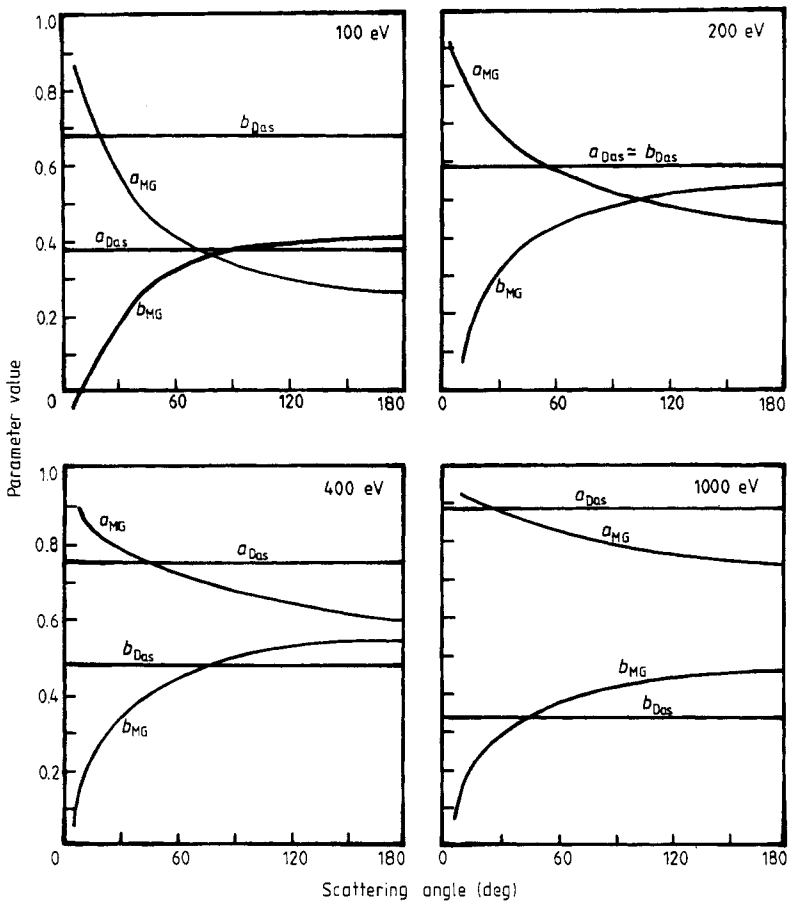

Figure 1. Variation of the parameters a_{Das}, b_{Das}, a_{MG} and b_{MG} with scattering angle at different energies.

hand, the MG results of Jhanwar *et al* (1982b) are in good agreement with the experimental data at small and intermediate angles. Thus at 100 eV, the present results at large angles are better than those obtained in the MG approximation. At 200 eV a similar situation occurs except that in the Das method the underestimate is now limited only up to 80° and the overestimate at higher angles increases with the increase of the scattering angle. At higher energies, although the Das results become satisfactory at small and intermediate angles, the overestimate at larger angles has increased further. The differential cross sections obtained by Das and his associates for e^-–H (Das and Biswas 1980) and e^-–He (Das *et al* 1981) elastic scattering also show similar trends. Thus the underestimate at small angles for the lower end of the intermediate energy range (100–1000 eV) and the overestimate at large angles for high energies of the range seems to be an associated characteristic of Das results.

Since the DCS obtained in the Das method at small angles are highly underestimated at 100 eV, the total elastic cross sections at 100 eV are also quite small (see table 1). As the energy increases, the difference between theory and experiment decreases. On the other hand, the total collisional cross sections obtained in the Das method and listed in table 2 are consistently too high in comparison to the experimental values

Table 1. The ratio $R = I_{theory}/I_{expt}$† for e^-–H_2 elastic scattering.

	100 eV		200 eV		400 eV		1000 eV	
Angle (deg)	Das[a]	MG[b]	Das	MG	Das	MG	Das	MG
5	0.29	0.97	0.39	0.92	0.61	0.98	0.90	1.03
10	0.29	0.94	0.50	0.95	0.76	0.98	1.01	1.06
15	0.36	0.96	0.65	0.98	0.87	1.00	1.01	1.05
20	0.47	0.99	0.75	0.99	0.90	0.99	0.90	0.93
30	0.64	0.97	0.81	0.94	0.84	0.90	1.00	1.01
40	0.71	0.94	0.81	0.92	0.84	0.89	1.21	1.19
50	0.82	1.02	0.82	0.90	0.96	0.98	1.16	1.09
70	0.76	0.85	0.87	0.86	1.12	1.03	1.34	1.15
90	0.81	0.76	1.04	0.88	1.09	0.89	1.33	1.05
110	0.91	0.69	1.14	0.83	1.10	0.94	1.41	1.05
130	0.98	0.62	1.15	0.76	1.40	0.98	1.52	1.08
σ_{theory}[c]	1.57	3.01	0.84	1.22	0.44	0.54	0.18	0.20
σ_{expt}	3.17	3.17	1.28	1.28	0.54	0.54	0.19	0.19

† Experimental data (absolute) are of van Wingerden *et al* (1977, 1980) up to 50° and beyond this angle are the data of Fink *et al* (1975) as renormalised by van Wingerden *et al.*

[a] I_{theory} are the present results of $I_{Das}(H_2)$.

[b] I_{theory} are the modified Glauber results obtained by Jhanwar *et al* (1982b).

[c] σ denotes the total elastic cross section. σ_{theory} are the present results in the Das method and those obtained by Jhanwar *et al* (1982a, b) while σ_{expt} are the values of van Wingerden *et al.*

Table 2. Total cross section (a_0^2), obtained by the optical theorem, for e^-–H_2 scattering.

Energy	Present	JKS[a]	SP[b]	H[c]	W[d]
100	10.23	9.57	10.65	9.14	9.01
150	7.83	7.45	7.89	7.07	7.13
200	6.44	6.11	—	5.96	5.76
300	4.78	4.52	4.55	4.50	4.36
400	3.84	3.61	3.61	3.57	3.45
500	3.22	3.02	—	3.04	2.97
700	2.45	2.29	—	—	2.28
1000	1.82	1.70	—	—	—

[a] JKS, Jhanwar *et al* (1982b).

[b] SP, theoretical results obtained by Srivastava and Pathak (1981) in their static corrected model along with the independent atom model.

[c] H, measurements of Hoffman *et al* (1982).

[d] W, measurements of van Wingerden *et al* (1980).

at all the energies under consideration. The MG results of Jhanwar *et al* (1982b) show much better agreement with the experimental data of Hoffman *et al* (1982) and van Wingerden *et al* (1977, 1980). The theoretical values obtained by Srivastava and Pathak (1981) for 300 and 400 eV are in good agreement with the experimental data but at 100 and 150 eV their values are even higher than the Das values.

Das and his associates did not compute total collisional cross sections for e^-–H and e^-–He scattering. Using their reported optimal values of a and b for these targets

(Das and Saha 1981) and the values of first Born, second Born and Ochkur exchange scattering amplitudes as calculated by Jhanwar *et al* (1982a) for H and He atoms and equation (1) of the present paper, we have obtained the real and imaginary parts of the Das forward scattering amplitudes for the scattering of electrons by the above mentioned atoms. The imaginary part is then converted via the optical theorem into total collisional cross sections. The only differences in the calculation of Das and Saha (1981) and Jhanwar *et al* (1982a) are slightly different values of the mean excitation energies used in the computation of f_{B2}. The parameters a and b, however, are quite insensitive to these. These results are reported in tables 3 and 4. Also included in these tables are other theoretical results and some of the available experimental data. The situation with respect to other theoretical and experimental data not included here, may be judged from the values listed by Jhanwar *et al* (1982a). Table 3 clearly shows that the real part of the Das amplitude in the forward direction is appreciably low, both for e^-–H and e^-–He scattering for the lower end of the energy range under consideration. A similar situation is observed for the e^-–H_2 scattering also. Furthermore, the real part of the Das amplitude increases with the increase in energy from 50–500 eV (see table 3) while the other theoretical and dispersion relation results, which are quite consistent with one another, decrease with the energy. The total cross sections obtained in the Das method (see table 4) overestimate the experimental and other theoretical data. This situation is again similar to that we have observed above for the case of e^-–H_2 scattering.

Finally, we conclude that the Das method yields satisfactory results for the DCS only at intermediate angles. The Das total cross section values for e^-–H_2 scattering are satisfactory for $E \geqslant 100$ eV. The real parts of the Das amplitude are drastically low particularly at small angles and energies while the imaginary parts at low angles are consistently too high. We, however, note that the technique proposed by Das, which does not need elaborate computation, is interesting. Some of the unsatisfactory aspects of the Das method could be improved by combining the eikonal–Born series (EBS) method and the Das method. The work in this direction is in progress and will be reported elsewhere.

Table 3. Real part of the forward elastic amplitude (in units of a_0).

E (eV)	Present	MG[a]	DR[b]	EBS[c]
e^-–H scattering				
50	0.908	3.11	2.90	—
100	1.11	2.39	2.37	—
200	1.20	1.94	1.94	—
400	1.23	1.64	1.64	—
e^-–He scattering				
50	0.470	2.75	—	—
100	0.730	2.01	1.91	1.91
200	0.837	1.58	1.71	1.54
500	0.895	1.25	1.29	1.24

[a] Obtained by Jhanwar *et al* (1982a) in the MG approximation.
[b] Dispersion relation results of de Heer *et al* (1977) for the hydrogen atom, and of Bransden and McDowell (1970) for the helium atom.
[c] Eikonal–Born series results of Byron and Joachain (1973).

Table 4. Total cross sections (in units of a_0^2).

	e^-–H scattering			e^-–He scattering		
E (eV)	Present	MG[a]	de Heer *et al* (1977)	Present	MG[a]	Expt[b]
50	15.0	10.1	10.3	12.1	3.37	6.19
100	8.76	6.85	6.85	6.99	3.89	3.96
200	4.96	4.18	4.18	3.80	2.76	2.55
400	2.73	2.43	2.43	—	1.71	1.62
500	—	2.03	—	1.70	1.44	1.36

[a] Obtained by Jhanwar *et al* (1982a).
[b] Experimental measurements of Kauppila *et al* (1981).

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