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Elastic scattering of electrons by hydrogen molecules in the modified Glauber approximation

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A modified Glauber approximation has been employed to investigate the elastic scattering of electrons by the hydrogen molecules in the intermediate-energy range (50 – 1000 eV). The exchange effects are included through the Glauber-Ochkur approximation. In general the effect of multiple scattering is found to be small and the differential cross sections agree very well with the absolute experimental data for $E \geq 100$ eV. The total cross sections for electron as well as positron scattering are also obtained via the optical theorem. The values are in good agreement with the available experimental data.

INTRODUCTION

Investigations of elastic scattering of electrons by light atoms, over the intermediate-energy range, have been successfully carried out by employing numerous approximate methods.[1] However, owing to additional complexity of the calculations, only some of these methods could be extended to the scattering of the electrons by even the simplest molecule,[2] e.g., H_2. The recent (second Born) calculations of Jhanwar *et al.*[2] for e-H_2 elastic scattering although does employ a molecular wave function (single center) but neglects the higher Born terms, which are found to be important for electron-atom scattering, particularly at the lower side of the intermediate-energy range. A way to partially account for these higher terms has been suggested by Gien[1] in the form of the modified Glauber approximation (MGA). In his MGA investigations on $e^{\pm}$-H and He atoms[1] Gien has demonstrated the importance of the higher-order terms. In MGA, special care is required to compute the forward scattering amplitudes owing to the occurence and exact cancellation of two divergences. Quite recently Jhanwar *et al.*[3] have developed analytical expressions for the forward MGA amplitude. The good agreement between their computed MGA total cross section (derived from the imaginary part of the forward amplitude) and experimental data further establishes the importance of the higher-order terms. Thus it is of interest to extend the application of MGA to the electron-molecule scattering. So far, no direct investigation of the molecular scattering in MGA has been performed. Indirectly, MGA has been used to investigate e-H_2 elastic scattering in the independent atom model (IAM). It is well known that in IAM the molecular scattering amplitude is expressible in terms of the atomic scattering amplitudes. MGA has been employed to obtain the hydrogenic scattering amplitude and thereby the IAM e-H_2 scattering amplitude.[4] It should, however, be noted that the effect of multiple scattering totally gets neglected in IAM investigations. Hence, it is desirable to employ MGA with a molecular wave function so that the multiple scattering effects can be incorporated. In this paper such an attempt has been made while investigating e-H_2 elastic scattering over 50 – 1000 eV.

We use a simple but fairly accurate two-center wave function for the ground state of H_2. We find that the use of separated atom approximation (SAA), which greatly simplifies the evaluation of the first Born amplitude without introducing appreciable errors,[5] is not enough to keep the second Born calculations tractable. Hence, we introduce an additional approximation and quite interestingly obtain the molecular second Born amplitude (f_{B2}) expressed in terms of the corresponding amplitude for the united atom limit of H_2, i.e., He atom. It may be noted that the first Born molecular amplitude (f_{B1}) is also expressible in terms of the amplitude for the united atom limit of H_2. Thus the present observations are at variance with that of the widely used IAM method in which the molecular scattering amplitude is expressed in terms of the amplitude for the separated atom limit of H_2. It is, therefore, evident that everything remaining the same, a comparison of present results with IAM results would provide information about the significance of the multiple scattering.

The differential cross section in MGA is calculated by assuming that like f_{B1} and f_{B2} the lesser important higher-order molecular scattering amplitudes are also expressible in terms of the amplitude for the united atom limit of H_2. In the computation of f_{B2}, which involves infinite summation, we retain the first term of the summation exactly and sum the remaining terms by using the closure relation after the various excitation energies have been replaced by an average excitation energy. The latter is so chosen that it reproduces the average (spherical) experimental value of the dipole polarizability in the closure relation. The contribution of exchange is included through the Glauber-Ochkur approximation.[6] Finally the averaged differential cross sections are obtained and compared with the experimental data.[7] We also employ the analytical expression developed by Jhanwar *et al.*[3] for the forward MGA amplitude of hydrogenic atom for computing the same for *e*-H_2 case. The imaginary part of the amplitude is then converted to the total cross section by using an optical theorem and is then compared with the available experimental data.

THEORY

The differential cross section (DCS) for the elastic scattering of the electrons by the hydrogen molecules averaged over all the orientations of the internuclear axis in modified Glauber (MG) and Glauber-Ochkur (GO) approximations is given by

$$\bar{I}_{H_2}(\theta)=|f_{MG}^{H_2}-g_{GO}^{H_2}|^2 , \tag{1}$$

where $f_{MG}^{H_2}$ and $g_{GO}^{H_2}$ are direct scattering amplitudes in modified Glauber and exchange scattering amplitudes in the Glauber-Ochkur approximation, repectively. Now

$$f_{MG}=f_G-f_{G2}+f_{B2} , \tag{2}$$

where f_G is the scattering amplitude in the Glauber approximation, f_{G2} is the second term of the Glauber series, and f_{B2} is the second Born scattering amplitude. Equation (2) may also be written as

$$f_{MG}=f_{B1}+f_{B2}+\sum_{n=3}^{\infty} f_{G_n} , \tag{3}$$

where f_{B1} is the first Born scattering amplitude and f_{G_n} is the *n*th term of the Glauber series. For the elastic scattering of electrons by the ground state of the hydrogen molecule, we have

$$f_{B1}=-\frac{1}{4\pi}\langle 0,\vec{k}_f\,|\,V\,|\,0,\vec{k}_0\rangle \tag{4}$$

and

$$f_{B2}=\frac{1}{32\pi^4}\sum_n \int d\frac{\vec{q}}{q^2-k_n^2-i\epsilon}\langle 0,\vec{k}_f\,|\,V\,|\,n,\vec{q}\,\rangle\langle n,\vec{q}\,|\,V\,|\,0,\vec{k}_0\rangle ,$$

with

$$|\,n,p\,\rangle=e^{i\vec{p}\cdot\vec{r}}\,|\,n\,\rangle , \tag{5}$$

where $\vec{k}_0$ and $\vec{k}_f$ are initial and final momentum vectors of the incident electron; $|\,0\,\rangle$ and $|\,n\,\rangle$ represent the initial and intermediate states of the molecule. The energy of the *n*th excited state E_n is given by (we express energy in the units of Rydberg and length in the units of Bohr radius)

$$E_n-E_0=k_0^2-k_n^2 . \tag{6}$$

The interaction potential V is given by

$$V(\vec{r}_1;\vec{r}_2,\vec{r}_3)=-\frac{2}{|\,\vec{r}_1-\vec{r}_A\,|}-\frac{2}{|\,\vec{r}_1-\vec{r}_B\,|}+\frac{2}{|\,\vec{r}_1-\vec{r}_2\,|}+\frac{2}{|\,\vec{r}_1-\vec{r}_3\,|} , \tag{7}$$

where $\vec{r}_1$ refers to the incident electron, $\vec{r}_2,\vec{r}_3,\vec{r}_A,\vec{r}_B$ are the coordinates of the bound electrons and the two nuclei *A* and *B* of the molecule, respectively.

To obtain f_{MG} and g_{GO}, we represent the hydrogen molecule by a simple but fairly accurate two-center wave function given by

$$\psi_0(\vec{r}_2,\vec{r}_3)=N[\phi_g(\vec{r}_2)\phi_g(\vec{r}_3)+C\phi_u(\vec{r}_2)\phi_u(\vec{r}_3)] , \tag{8}$$

where the gerade and ungerade orbitals are given by

$$\phi_{g,u}(\vec{r}_i)=N_{g,u}[v(\vec{r}_{iA})\pm v(\vec{r}_{iB})] , \qquad (9)$$

with

$$v(\vec{r}_i)=\left[\frac{Z^3}{\pi}\right]^{1/2} e^{-Zr_i} \qquad (10)$$

and

$$N_{g,u}^2=\frac{1}{2(1\pm S)} . \qquad (11)$$

Taking the midpoint of the molecule as the origin we have

$$\vec{r}_A=-\vec{r}_B=\vec{R} , \qquad (12)$$

where $2R$ is the equilibrium internuclear distance, and the overlap integral

$$S=(1+2ZR+\tfrac{4}{3}Z^2R^2)e^{-2ZR} . \qquad (13)$$

For $R=0.7$, the variational parameters Z and C are equal to 1.2005 and -0.5814, respectively. The normalization constant N is equal to $(1+C^2)^{-1/2}$.

Putting (8) in (4), it is easy to show that in SAA, the separated atom approximation (neglect of overlap integrals),[5]

$$f_{B1}^{\mathrm{H}_2}=2\cos(\vec{K}\cdot\vec{R})f_{B1}^{\mathrm{H}}(Z) , \qquad (14)$$

where $\vec{K}=\vec{k}_0-\vec{k}_f$, and $f_{B1}^{\mathrm{H}}(Z)$ is the scattering amplitude in the first Born approximation for the electron elastically scattered by a hydrogenlike atom represented by (10). It has been shown[5] that (14) is at the maximum only 4% different from the exact result for $f_{B1}^{\mathrm{H}_2}$. Hence, SAA is satisfactory in the first Born approximation and we shall assume it to be satisfactory for all the terms of f_{MG} and g_{GO}. It is well known[4] that if we work in the independent atom model and use the first Born approximation for the two atoms we again get (14).

Now we proceed to obtain $f_{B2}^{\mathrm{H}_2}$. Considering the molecule as composed of two atoms we may rewrite (7) as

$$V(\vec{r}_1;\vec{r}_2,\vec{r}_3)=V_A(\vec{r}_2)+V_B(\vec{r}_3) , \qquad (15)$$

with

$$V_A(\vec{r}_2)=-\frac{2}{|\vec{r}_1-\vec{r}_A|}+\frac{2}{|\vec{r}_1-\vec{r}_2|} \qquad (16)$$

and

$$V_B(\vec{r}_3)=-\frac{2}{|\vec{r}_1-\vec{r}_B|}+\frac{2}{|\vec{r}_1-\vec{r}_3|} . \qquad (17)$$

Putting (16) and (17) in (5) we get

$$f_{B2}^{\mathrm{H}_2}=f_{AA}+f_{BB}+f_{AB}+f_{BA} , \qquad (18)$$

where

$$f_{AA}=\frac{1}{32\pi^4}\sum_n\int\frac{d\vec{q}}{q^2-k_n^2-i\epsilon}\langle 0,\vec{k}_f\,|\,V_A\,|\,n,\vec{q}\,\rangle\langle n,\vec{q}\,|\,V_A\,|\,0,\vec{k}_0\rangle , \qquad (19)$$

$$f_{AB}=\frac{1}{32\pi^4}\sum_n\int\frac{d\vec{q}}{q^2-k_n^2-i\epsilon}\langle 0,\vec{k}_f\,|\,V_A\,|\,n,\vec{q}\,\rangle\langle n,\vec{q}\,|\,V_B\,|\,0,\vec{k}_0\rangle , \qquad (20)$$

and similar expressions for f_{BB} and f_{BA}. Evidently both (19) and (20) represent double scattering. However, f_{AA} is for the process in which the incident electron is scattered twice by the same atom A, while in f_{AB} the incident electron is first scattered by the atom B and then by the atom A. Similar interpretation is assigned to the terms f_{BB} and f_{BA}. Although the terms f_{AA} and f_{BB} were included in the investigation of Jhanwar *et al.*,[4] the double scattering terms f_{AB} and f_{BA} and similar higher multiple scattering terms were not taken into consideration. When we speak about multiple scattering in the future, we shall mean only those scattering processes in which the incident electron is scattered by both the atoms in succession as represented by f_{AB}, etc. As expected, the second Born approximation for the molecule includes such double scattering terms. Similarly, $f_{G_n}(n>3)$ for the molecule includes all the higher multiple scattering terms.

To evaluate f_{AA}, we employ the Bethe integral in (19) to integrate over $\vec{r}_1$ and obtain

$$f_{AA}=\frac{2}{\pi^2}\sum_n\int\frac{d\vec{q}}{K_2^2K_3^2(q^2-k_n^2-i\epsilon)}\langle 0|-e^{i\vec{K}_2\cdot\vec{R}}+e^{i\vec{K}_2\cdot\vec{r}_2}|n\rangle\langle n|-e^{i\vec{K}_3\cdot\vec{R}}+e^{i\vec{K}_3\cdot\vec{r}_2}|0\rangle , \qquad (21)$$

with

$$\vec{K}_2=\vec{q}-\vec{k}_f$$

and

$$\vec{K}_3=\vec{k}_0-\vec{q}\ . \tag{22}$$

The first term of the above series is retained exactly and the rest of the terms are summed by closure. A similar procedure is adopted to evaluate f_{BB}. Now taking $f_{AA}+f_{BB}$ and proceeding to the separated atom limit we obtain

$$\begin{aligned} f_{AA}+f_{BB}=\frac{4}{\pi^2}\int\frac{d\vec{q}}{K_2^2K_3^2(q^2-p^2-i\epsilon)}&\{\cos(\vec{K}\cdot\vec{R})[1+\mathscr{I}(K)]-\cos(\vec{K}_2\cdot\vec{R})\cos(\vec{K}_3\cdot\vec{R})[\mathscr{I}(K_2)+\mathscr{I}(K_3)]\}\\ &+\frac{4}{\pi^2}\int\frac{d\vec{q}}{K_2^2K_3^2}\left[\frac{1}{q^2-k_0^2-i\epsilon}-\frac{1}{q^2-p^2-i\epsilon}\right]\\ &\times\{\cos(\vec{K}\cdot\vec{R})-\cos(\vec{K}_2\cdot\vec{R})\cos(\vec{K}_3\cdot\vec{R})[\mathscr{I}(K_2)+\mathscr{I}(K_3)\\ &+\mathscr{I}(K_2)\mathscr{I}(K_3)]\}\ . \end{aligned}\tag{23}$$

where

$$\mathscr{I}(s)=\frac{Z^3}{\pi}\int e^{i\vec{s}\cdot\vec{r}}e^{-2Zr}d\vec{r}\ , \tag{24}$$

and $p^2=k_0^2-\Delta$, Δ being the mean excitation energy. As was mentioned earlier, the value of Δ is so chosen that it reproduces the average experimental value of dipole polarizability α_d of H_2 in the closure approximation.[8] Thus with $Z=1.2005$ and $\alpha_d=5.18$ we obtain Δ equal to 1.08. The integrals in (23) containing $\cos(\vec{K}_2\cdot\vec{R})\cos(\vec{K}_3\cdot\vec{R})$ are difficult to evaluate, hence a simple approximation is introduced here. Let us consider the integral

$$I=\int d\vec{q}\cos(\vec{K}_2\cdot\vec{R})\cos(\vec{K}_3\cdot\vec{R})T(\vec{q},\vec{k}_0,\vec{k}_f)\ .$$

At high energies, the cosine functions are highly oscillating. If $T(\vec{q},\vec{k}_0,\vec{k}_f)$ is assumed to be slowly varying with $\vec{q}$, then the major contribution to the integral comes from those values of $\vec{q}$ for which oscillations are very slow. The oscillations in, for example, $\cos(\vec{K}_2\cdot\vec{R})$ vanish for $\vec{q}=\vec{k}_f$ yielding $\vec{K}_2=0$ and $\vec{K}_3=\vec{K}$. Making this substitution in $\cos(\vec{K}_2\cdot\vec{R})$ and $\cos(\vec{K}_3\cdot\vec{R})$ (phase terms) in (23) we obtain

$$\begin{aligned} f_{AA}+f_{BB}=2\cos(\vec{K}\cdot\vec{R})\Bigg[&\frac{2}{\pi^2}\int\frac{d\vec{q}}{K_2^2K_3^2(q^2-p^2-i\epsilon)}[1-\mathscr{I}(K_2)-\mathscr{I}(K_3)+\mathscr{I}(K)]\\ &+\frac{2}{\pi^2}\int\frac{d\vec{q}}{K_2^2K_3^2}\left[\frac{1}{q^2-k_0^2-i\epsilon}-\frac{1}{q^2-p^2-i\epsilon}\right]\\ &\times[1-\mathscr{I}(K_2)-\mathscr{I}(K_3)+\mathscr{I}(K_2)\mathscr{I}(K_3)]\Bigg]\ . \end{aligned}\tag{25}$$

The integrals of (25) are evaluated by the Feynmann technique. The expressions are well known and need not be given here. It may, however, be noted that the content of the large square bracket is equal to $f_{B2}^{\mathrm{H}}(Z)$. A similar procedure is employed to evaluate f_{AB}, from (20) we obtain in SAA

$$f_{AB}=\frac{2}{\pi^2}\int\frac{d\vec{q}}{K_2^2K_3^2}\left[\frac{1}{q^2+k_0^2-i\epsilon}-\frac{1}{q^2-p^2-i\epsilon}\right][-e^{-i\vec{K}_2\cdot\vec{R}}+\cos(\vec{K}_2\cdot\vec{R})\mathscr{I}(K_2)][-e^{i\vec{K}_3\cdot\vec{R}}+\cos(\vec{K}_3\cdot\vec{R})\mathscr{I}(K_3)]$$
$$+\frac{2}{\pi^2}\int\frac{dq}{K_2^2K_3^2(q^2-p^2-i\epsilon)}[e^{-i(\vec{K}_2-\vec{K}_3)\cdot\vec{R}}-e^{-i\vec{K}_2\cdot\vec{R}}\cos(\vec{K}_3\cdot\vec{R})\mathscr{I}(K_3)-e^{i\vec{K}_3\cdot\vec{R}}\cos(\vec{K}_2\cdot\vec{R})\mathscr{I}(K_2)$$
$$+\cos(\vec{K}_2\cdot\vec{R})\cos(\vec{K}_3\cdot\vec{R})\mathscr{I}(K_2)\mathscr{I}(K_3)-2N^2C\sin(\vec{K}_2\cdot\vec{R})\sin(\vec{K}_3\cdot\vec{R})\mathscr{I}(\vec{K}_2)\mathscr{I}(K_3)]\,. \tag{26}$$

An expression similar to (26) is obtained for f_{BA}. Again in phase terms of $f_{AB}+f_{BA}$ we set $\vec{K}_2=0$ and $\vec{K}_3=\vec{K}$ and obtain

$$f_{AB}+f_{BA}=\cos(\vec{K}\cdot\vec{R})f'_{B2}(Z)\,, \tag{27}$$

with

$$f'_{B2}(Z)=\frac{4}{\pi^2}\int\frac{d\vec{q}}{K_2^2K_3^2}\left[\frac{1}{q^2-k_0^2-i\epsilon}-\frac{1}{q^2-p^2-i\epsilon}\right][-1+\mathscr{I}(K_2)]$$
$$\times[-1+\mathscr{I}(K_3)]+\frac{4}{\pi^2}\int\frac{d\vec{q}}{K_2^2K_3^2(q^2-p^2-i\epsilon)}[1-\mathscr{I}(K_2)-\mathscr{I}(K_3)+\mathscr{I}(K_2)\mathscr{I}(K_3)]\,. \tag{28}$$

Putting (25) and (27) in (18) we get

$$f_{B2}^{H_2}=\cos(\vec{K}\cdot\vec{R})[2f_{B2}^{H}(Z)+f'_{B2}(Z)]\,. \tag{29}$$

The difference in the structures of (14) and (29) arises due to double scattering represented by the term $f'_{B2}(Z)$.

It is well known that the united atom limit ($R=0$) of the hydrogen molecule is the helium atom. In this limit $\psi_0(\vec{r}_2,\vec{r}_3)$ given by (8) reduces to $v(\vec{r}_2)v(\vec{r}_3)$. Therefore, setting $R=0$ in (14) and (29) we obtain

$$f_{B1}^{\mathrm{He}}(Z)=2f_{B1}^{H}(Z) \tag{30}$$

and

$$f_{B2}^{\mathrm{He}}(Z)=2f_{B2}^{H}(Z)+f'_{B2}(Z)\,, \tag{31}$$

where $f_{B1}^{\mathrm{He}}(Z)$ and $f_{B2}^{\mathrm{He}}(Z)$ are the scattering amplitudes in the first and the second Born approximations, respectively, for an electron scattered by a helium atom represented by $v(\vec{r}_2)v(\vec{r}_3)$. Hence (14) and (29) reduce to

$$f_{B1}^{H_2}=\cos(\vec{K}\cdot\vec{R})f_{B1}^{\mathrm{He}}(Z) \tag{32}$$

and

$$f_{B2}^{H_2}=\cos(\vec{K}\cdot\vec{R})f_{B2}^{\mathrm{He}}(Z)\,. \tag{33}$$

On the assumption that similar relations hold between $f_{G_n}^{H_2}$ and $f_{G_n}^{\mathrm{He}}(Z)$ for $n\geq 3$, we take

$$f_{\mathrm{MG}}^{H_2}=\cos(\vec{K}\cdot\vec{R})\left[f_{B1}^{\mathrm{He}}(Z)+f_{B2}^{\mathrm{He}}(Z)+\sum_{n\geq 3}^{\infty}f_{G_n}^{\mathrm{He}}(Z)\right]. \tag{34a}$$

Using (2) and (3), Eq. (34a) may be rewritten as

$$f_{\mathrm{MG}}^{H_2}=\cos(\vec{K}\cdot\vec{R})[f_{G}^{\mathrm{He}}(Z)-f_{G2}^{\mathrm{He}}(Z)+f_{B2}^{\mathrm{He}}(Z)]\,, \tag{34b}$$

where the terms of the parenthesis are given by

$$f_X^{\mathrm{He}}(Z)=2f_X^{H}(Z)+f'_X(Z)\,. \tag{35}$$

The expressions for $f_G^H(Z)$, $f_{G2}^H(Z)$, and $f_{B2}^H(Z)$ are well known. $f'_G(Z)$ is evaluated following Sur *et al.*,[9] and the expressions for $f'_{G2}(Z)$ and $f'_{B2}(Z)$ are given[3] by

$$f'_{G2}(Z)=2i[I(\alpha,\beta)-\alpha^2D_\alpha I(\alpha,\beta)$$
$$-\beta^2D_\beta I(\alpha,\beta)+\alpha^2\beta^2D_\alpha D_\beta I(\alpha,\beta)] \tag{36}$$

and

$$f'_{B2}(Z)=8[A_{k_0}(\alpha,\beta)-\alpha^2D_\alpha A_{k_0}(\alpha,\beta)$$
$$-\beta^2D_\beta A_{k_0}(\alpha,\beta)+\alpha^2\beta^2D_\alpha D_\beta A_{k_0}(\alpha,\beta)]\,, \tag{37}$$

where D_α indicates the partial differential $\partial/\partial(\alpha^2)$ and $\alpha=\beta=2Z$. Also we have defined

$$I(\alpha,\beta)=\frac{1}{\pi k_0}\int\frac{d\vec{q}}{(|\vec{K}-\vec{q}|^2+\alpha^2)(q^2+\beta^2)}\,, \tag{38}$$

where $\vec{K}$ and $\vec{q}$ are two-dimensional vectors perpendicular to the Z axis. By the usual technique one obtains

$$I(\alpha,\beta)=\frac{2}{k_0 P}\ln\left[\frac{P+K^2+\alpha^2+\beta^2}{2\alpha\beta}\right], \tag{39}$$

with

$$P^2=(K^2+\alpha^2+\beta^2)^2-4\alpha^2\beta^2\,.$$

Note that for $\alpha=0$ and/or $\beta=0$, $I(\alpha,\beta)$ diverges. However, as mentioned by Yates,[10] for the particular combination of integrals appearing in $f_{G2}^{\mathrm{H}}(Z)$, both the infinities cancel each other exactly. Similarly, we have defined

$$A_p(\alpha,\beta)=\frac{1}{2\pi^2}\int\frac{d\vec{q}}{(q^2-p^2-i\epsilon)(K_2^2+\alpha^2)(K_3^2+\beta^2)}\,. \tag{40}$$

The value of $f_{\mathrm{MG}}^{\mathrm{H}_2}$ in the forward direction ($\vec{K}=0$) is obtained by using the expressions for the terms of (34b) in the forward direction. An analytical expression for

$$[f_G^{\mathrm{H}}(Z)-f_{G2}^{\mathrm{H}}(Z)]$$

in the forward direction, recently developed by us,[3] has been used to obtain

$$[f_G^{\mathrm{He}}(Z)-f_{G2}^{\mathrm{He}}(Z)]_{K=0}\,.$$

The expression for $f_{B2}^{\mathrm{He}}(Z)$ is well known.

Now, like the direct Glauber amplitude, the Glauber-Ochkur (GO) exchange amplitude for H_2 may also be assumed to be given by

$$g_{\mathrm{GO}}^{\mathrm{H}_2}=\cos(\vec{K}\cdot\vec{R})g_{\mathrm{GO}}^{\mathrm{He}}\,, \tag{41}$$

where $g_{\mathrm{GO}}^{\mathrm{He}}$ is the corresponding GO exchange amplitude for the helium atom, the expression for which may be obtained following Dewangan and Khayrallah[6] is given by

$$g_{\mathrm{GO}}^{\mathrm{He}}=\frac{\alpha^2\Gamma(1-i\eta)}{(2\alpha)^{i\eta}k_0^2}\left[\frac{i\eta(\alpha^2-K^2)-2\alpha^2}{(\alpha^2+K^2)^{2-i\eta}}\right], \tag{42}$$

where $\eta=-1/k_0$.

Finally, the substitution of (34b) in (1) and averaging over all the orientations of the molecular axis yields

$$I_{\mathrm{H}_2}(\theta)=\tfrac{1}{2}\left[1+\frac{\sin 2KR}{2KR}\right]|f_{\mathrm{MG}}^{\mathrm{He}}(Z)-g_{\mathrm{GO}}^{\mathrm{He}}(Z)|^2\,. \tag{43}$$

Furthermore, the imaginary parts of the forward amplitudes of

$$[f_{\mathrm{MG}}^{\mathrm{H}_2}(Z)-g_{\mathrm{GO}}^{\mathrm{H}_2}(Z)]_{K=0}$$

for electrons and

$$[f_{\mathrm{MG}}^{\mathrm{H}_2}(Z)]_{K=0}$$

for positrons are converted into total scattering cross sections through optical theorem.

CALCULATIONS, RESULTS, AND DISCUSSION

We have calculated $I_{\mathrm{H}_2}(\theta)$ from (43) for the incident energies varying from 50 to 1000 eV. In Figs. 1 to 3 our results for 50, 100, and 400 eV are shown along with the absolute experimental data[7] of van Wingerden *et al.* and renormalized data of Fink *et al.* and Lloyd *et al.* Except at 50 eV, the present results for 100 and 400 eV, and also for 200 and 1000 eV (not shown), are in good agreement with the experimental data. At 50 eV our MG results for e-H_2 elastic scattering overestimates the differential cross sections. It is well known[1] that methods such as MG and the

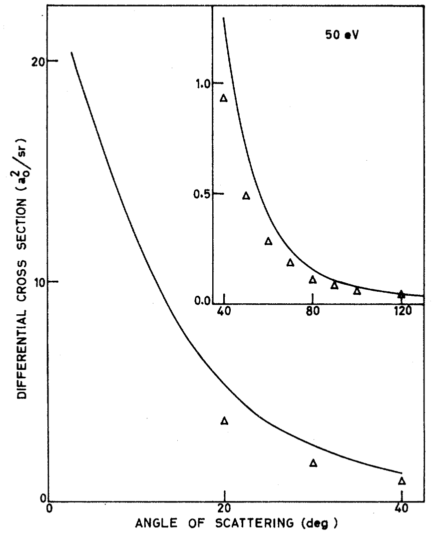

FIG. 1. Differential cross sections for electrons elastically scattered by hydrogen molecules for incident energy 50 eV; △: experimental results of Lloyd *et al.*

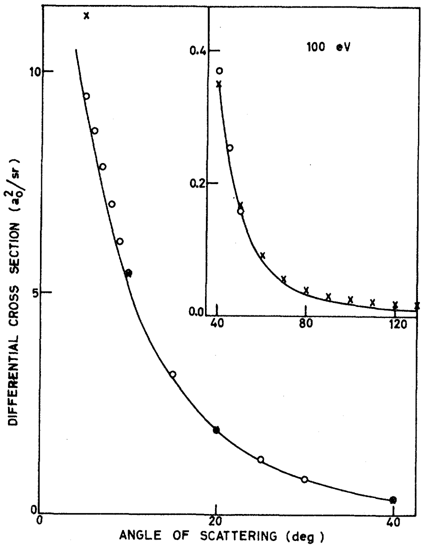

FIG. 2. Same as Fig. 1 for 100 eV; ○: experimental results of van Wingerden *et al.*; ×: experimental results of Fink *et al.* as renormalized by van Wingerden *et al.*

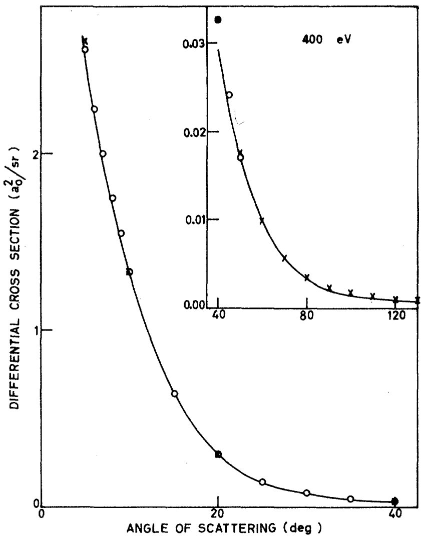

FIG. 3. Same as Fig. 2 but for 400 eV.

eikonal-Born series for *e*-He scattering become less reliable as the incident energy decreases below 100 eV. Thus the poor agreement between our MG results and experiments at 50 eV is not unexpected.

To examine the effect of multiple scattering we have shown in Table I the values of the ratio $I_{\mathrm{MG}}/I_{\mathrm{IAM}}$ as a function of the scattering angle θ at different impact energies. The values of I_{IAM} are taken from Jhanwar *et al.*[4] Equations (34b) and (41) show that the total scattering amplitude, including exchange, may be written as

$$F_{\mathrm{MG}}=\cos(\vec{\mathrm{K}}\cdot\vec{\mathrm{R}})(F_{\mathrm{IAM}}+f')\ ,$$

where f' arises due to multiple scattering. Hence we get

$$\frac{I_{\mathrm{MG}}}{I_{\mathrm{IAM}}}=1+\frac{\Delta}{|F_{\mathrm{IAM}}|^2}\ ,$$

where

$$\Delta=2\,\mathrm{Re}(F_{\mathrm{IAM}}f')+|f'|^2\ .$$

TABLE I. Ratios of differential cross sections in MGA to that in IAM for electrons elastically scattered by hydrogen molecules for incident energies 50–1000 eV.

Angle (deg)	50 eV	100 eV	200 eV	400 eV	1000 eV
5	0.92	0.95	0.99	1.01	1.00
10	0.91	0.94	0.97	0.98	0.99
15	0.90	0.93	0.95	0.97	0.98
20	0.89	0.91	0.94	0.96	0.99
30	0.83	0.89	0.92	0.96	1.00
40	0.90	0.88	0.91	0.97	1.01
50	0.92	0.86	0.91	0.98	1.03
60	0.94	0.85	0.91	0.99	1.03
70	0.96	0.84	0.91	1.01	1.04
80	0.98	0.83	0.91	1.02	1.05
100	1.01	0.79	0.90	1.04	1.05
120	1.03	0.75	0.90	1.06	1.05
140	1.04	0.72	0.90	1.07	1.06
160	1.05	0.70	0.89	1.08	1.06
180	1.05	0.69	0.89	1.08	1.06

TABLE II. Total cross section (in units of a_0^2) for $e^{\pm}$-H_2 scattering.

	For electron				For positron	
	Present	Ref. 12	Ref. 13	Ref. 14	Present	Ref. 14
100	9.57	9.80	9.01	9.14	9.52	9.57
150	7.45		7.13	7.07	7.43	
200	6.11		5.76	5.96	6.10	6.11
300	4.52		4.36	4.50	4.51	4.52
400	3.61		3.45	3.57	3.61	3.57
500	3.02		2.97	3.04	3.02	3.07
700	2.29		2.28		2.29	
1000	1.70				1.70	

The magnitude of $\Delta/|F_{\mathrm{IAM}}|^2$ is expected to decrease with the increase of the incident energy. Our results in Table I clearly show such a behavior at all scattering angles for $E \geq 100$ eV. We also notice that at 100 and 200 eV, Δ remains negative throughout, and the magnitude of $\Delta/|F_{\mathrm{IAM}}|^2$ continously increases with the scattering angle. However, at higher impact energies as well as at 50 eV, Δ passes through zero at some intermediate scattering angle. Because of this, at large angles, the effect of multiple scattering for 50 eV is smaller than those for higher impact energies. A simple explanation for this type of variation of $\Delta/|F_{\mathrm{IAM}}|^2$ with energy and angle remains obscure. However, in general, the values of the ratio is close to unity indicating that the effect of multiple scattering is small, in agreement with the findings of Hayashi and Kuchitsu[11] who found the effect of double scattering for H_2 to be less than 3%. We also note that at large angles I_{MG} is not in as good agreement with the experimental data as I_{IAM} is. This may be due to the use of SAA and the replacement of $\vec{K}_2$ by zero and $\vec{K}_3$ by $\vec{K}$ in the phase terms of (23) and (26).

Since at 50 eV MGA highly overestimates the differential cross sections, we have shown in Table II total cross sections only for $E \geq 100$ eV which may be regarded as reliable. We have obtained the total cross sections from the imaginary part of the forward elastic scattering amplitude via optical theorem, and have compared them with experimental data which have become available only recently.[12-14] There are no other theoretical values available for comparison. Table II shows that our values for the electron as well as positron scatterings are in good agreement with the experimental data. Our values for the electrons are consistently slightly higher than the experimental values of van Wingerden *et al.*[13] and Hoffman *et al.*,[14] the data of Hoffman *et al.* being closer to our values at all energies except at 150 eV. The maximum difference between our values and those of van Wingerden *et al.* is about 5% in 100–700 eV range; the agreement of 700 eV is almost perfect. The agreement between our results and experimental data of Hoffman *et al.* for positron scattering is again very good.

It may also be observed from Table II that the ratios $R=(Q_T)_{e\pm}/(Q_T)_e$ are close to unity theoretically as well as experimentally. However, theoretical values of R are always less than or equal to unity, whereas experimental values as obtained from the data of Hoffmann *et al.* are always greater than or equal to one. We note that the experimentally[14-15] determined ratio R for other targets such as He, Ne Ar, Kr, and N_2 all exhibit the same trend as that given by our theory. One of the sources of error in the experimental measurement of the total scattering cross section[15] is the partial neglect of the small-angle elastic scattering. The error, being different for electrons and positrons, may be responsible for giving the opposite experimental trend for H_2.

Finally we conclude that the modified Glauber approximation can be employed with success to obtain differential and total cross sections for electron-molecule scattering in the intermediate-energy range. Hence the extension of present investigation, preferably with a better exchange approximation to other molecular scatterings, will be of interest.

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