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Polarization effects in the elastic scattering of electrons by molecular hydrogen

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The elastic differential cross section of electrons from molecular hydrogen has been calculated in the independent-atom model using the Glauber approximation for both direct and exchange scattering amplitudes. Polarization effects have been considered through the modified Glauber amplitude for the direct scattering. For the exchange amplitude the result obtained by Franco and Halpern has been used. Numerical results for various incident electron energies have been carried out. The polarization contribution has been found to have negative effects in bringing the calculated results close to the experimental values.

INTRODUCTION

The experimental investigations of Van Wingarden *et al.*[1] on the elastic differential scattering cross section (DSC) of electrons from molecular hydrogen have generated great interest for theoretical investigations of the same problem in various approximation schemes.[2–7] The less expensive eikonal and related approximations[8–11] have also been used for this study.

The present authors have recently[12] derived the DSC for the e^--H_2 molecule in the independent atom model (IAM). In those calculations the polarization effects have not been taken into consideration. The valence bond effects have been incorporated by taking the value of the charge z in the atomic orbital e^{-zr} (we use atomic units throughout) to be 1.2. Further, for the numerical calculations the exchange amplitude as given by Khayrallah[13] has been uesd. This has been recently shown by Franco and Halpern[14] to be incorrect.

In the present paper we incorporate the polarization effects along with the correct exchange amplitude of Franco and Halpern.[14] The polarization effects have been included through the modified Glauber (MG) amplitude of Gien.[15] After submitting our results for publication it has been brought to our notice that similar investigations have recently been made by Jhanwar *et al.*[16] The DSC expression used by these authors differs from the present one, even though it does not have the unphysical behavior of not containing the exchange term in the limiting case where the internuclear distance (R) tends to zero. This type of incorrect behavior was the feature of the result obtained by Srivastava *et al.*[17] Using the well-known[18] result that DSC for e^-- H_2 molecule scattering is given by $|f-g|^2$, we derived in Glauber approximation the DSC expression [see Eq. (1) below] in terms of atomic scattering amplitudes. Here f and g are the molecular direct and exchange scattering amplitudes, respectively. On the other hand, Jhanwar *et al.*[16] used Born and Ochkur[19] approximations in relating the scattering amplitudes f and g to the corresponding atomic scattering amplitudes f^d and f^e. They obtained their result for DSC to be

$$2\,|f^d-\tfrac{1}{2}f^e|^2[1+j_0(qR)]\ ,$$

where j_0 is the spherical Bessel function of order zero and q is the momentum transfer. Gien[20] has shown the inadequacy of the Ochkur approximation for eikonal theory.

We considered both the direct and exchange scatterings in Glauber[21] approximation and also both the arbitrary z direction ($q_z \neq 0$) [denoted as unrestricted Glauber approximation (URG)] and the straight-line approximation ($q_z=0$) [called as restricted Glauber approximation (RG)] for the exchange scattering amplitude. Further, we compare the results obtained by including the polarization with the unpolarized results.

We give below the theoretical formulas used for the present calculations, and our numerical DSC results for various incident electron energies and compare them with the available experimental values.[1,22–24] We also present the integrated cross sections for various energies.

THEORY

In IAM the elastic DSC for the scattering of electrons from molecular hydrogen is given by Eq. (14) of Ref. 12 as

$$\left[\frac{d\sigma}{d\Omega}\right]_{e^{-}\text{-H}_2}=2\,|f^d-f^e|^2[1+j_0(qR)]\ . \tag{1}$$

For f^d we used the MG result of Gien[15] as

$$f^d=f_G-f_{G_2}+f_{B_2}\ . \tag{2}$$

The full direct Glauber scattering amplitude f_G is given by Eq. (28a) of Thomas and Gerjuoy[25] with the proper modification of z. The second Glauber f_{G_2} and the second Born f_{B_2} direct amplitudes are given by Eqs. (27), (32), (33a), and (33b) of Gien,[26] again modifying properly the value of z. The exchange amplitude f^e has been given by [with a proper modification of Eq. (27), Ref. 14, to include the binding effects]

$$f^e=\frac{8\pi\eta e^{\pi\eta/2}}{k_i^{2+i\eta}\sinh\pi\eta}\,\frac{\left[\lambda-\dfrac{i_q^2}{2k_i}\right]^{-i-i\eta}}{(\lambda^2+q^2)2-i\eta}\times\left[-i\eta(\lambda^2+q^2)+2\lambda(i\eta-1)\left[\lambda-\frac{iq^2}{2k_i}\right]\right], \tag{3}$$

where $\lambda=2z$, $\eta=1/k_i$, and k_i is the momentum of the incident electron for the URG approximation. The expression for RG is obtained by taking the limit $q_z=0$ in Eq. (3). The integrated cross section is given by

$$\sigma_t=\int\left[\frac{d\sigma}{d\Omega}\right]_{e^{-}\text{-H}_2}d\Omega\ . \tag{4}$$

RESULTS

The elastic DSC has been evaluated for incident electron energies of 50, 200, 1000, and 2000 eV. The molecular binding effects, as pointed out by Pauling and Wilson,[27] have been incorporated by taking $z=1.193$ in the exponent of the atomic orbital e^{-zr}. The results are presented in Figs. 1–3. For comparison we have also plotted the other theoretical and experimental results in these figures. Comparing the results obtained by including the polarization with the corresponding unpolarized ones one can notice on the whole that the latter results are in better agreement with the experimental values than the former ones.

From a comparison of RG and URG results we notice that the difference between the two is considerable for low- and medium-energy incident electrons. At high energies the difference almost vanishes. As expected the straight-line approximation gives results closer to experimental values at small angles of scattering. As the angle of scattering increases the results with nonzero q_z are in better agreement with experimental values than

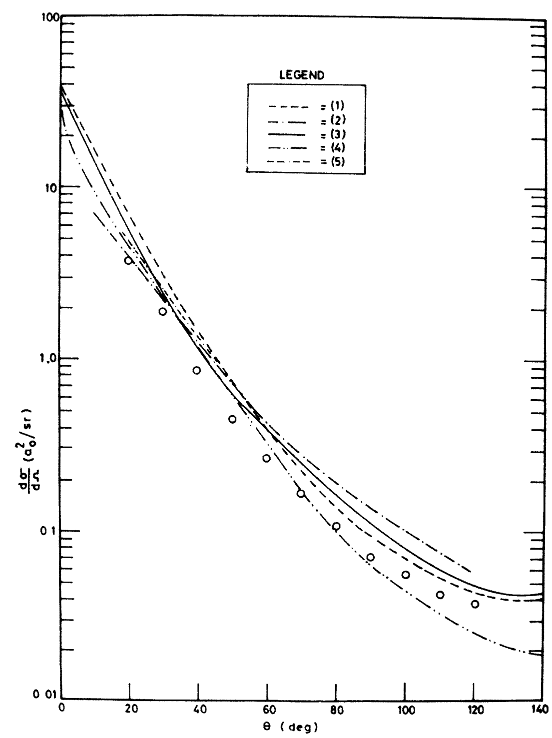

FIG. 1. Differential cross section of e^{-}-H_2 for 50-eV incident electrons in units of a_0^2/sr. Curve (1): Glauber with polarization for direct and URG exchange, curve (2): Polarized Born and Ochkur exchange, curve (3): Glauber with polarization for direct and Ochkur exchange, curve (4): Glauber direct and URG exchange, curve (5): Glauber with polarization for direct and RG exchange, (○): Experimental results of Lloyd *et al.* (Ref. 24).

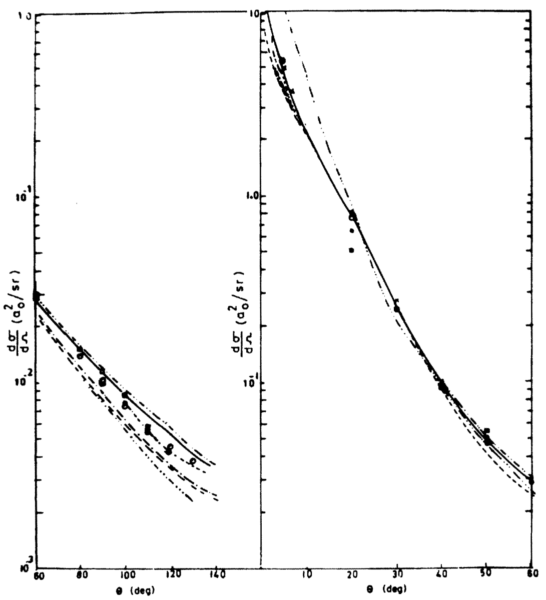

FIG. 2. DSC of e^--H_2 for 200 eV. Glauber with polarization and URG for exchange ——; Glauber for direct and URG for exchange —··—··—; Glauber for direct and RG for exchange —·—·—; Truhlar and coworkers from Ref. 1 —···—···—···—; Khare and coworkers from Refs. 3 and 1 ·——·——·——. Experimental data: ×, Van Wingarden *et al.* (Ref. 1); ○, Fink *et al.* (Ref. 22); ●, Williams *et al.* (Ref. 23); ■, Lloyd *et al.* (Ref. 24).

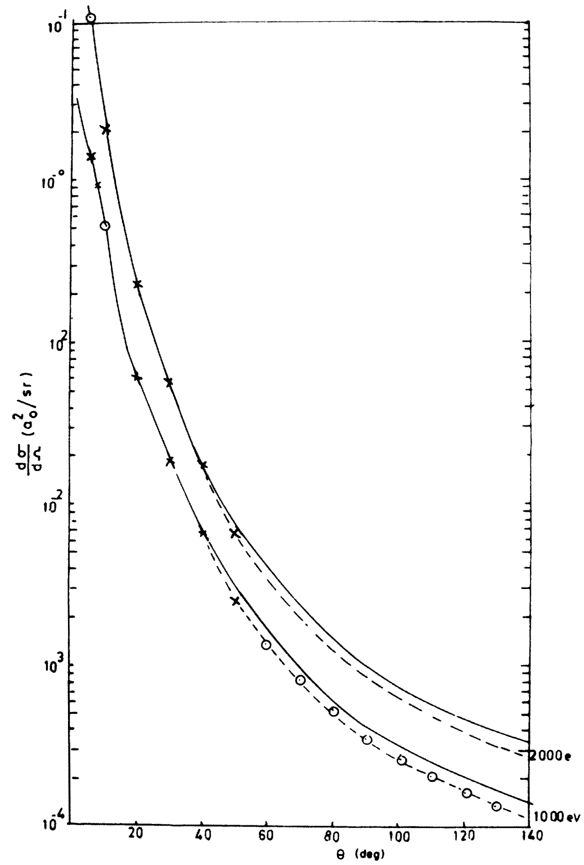

FIG. 3. DSC of e^--H_2 for 1000 and 2000 eV. Notation is the same as in Fig. 2.

those with $q_z=0$. The DSC results at large angles of scattering for medium-energy incident electrons are underestimated with $q_z=0$. This feature decreases as the energy of incident electrons increases. To compare the Glauber and Ochkur approximations, we have also calculated the DSC for 50-eV incident electron energy with the MG approximation for the direct amplitude along with

TABLE I. e^--H_2 integrated cross sections in a_0^2 units. Numbers in the parentheses denote the exponent of 10.

Energy (eV)	Experiment (Ref. 1)	MG direct and URG exchange	Khare and co-workers	Truhlar
30		28.14	15[a]	
50		10.65	7.15[a]	
100	3.17	3.38	2.72[b]	3.65
200	1.28	1.25	1.22[b]	1.85
400	5.43(−1)	5.27(−1)	5.80(−1)[b]	
500	4.20(−1)	4.06(−1)	4.60(−1)[b]	
700	2.60(−1)	2.78(−1)	3.20(−1)[b]	
1000	1.86(−1)	1.86(−1)		
2000	9.70(−2)	9.14(−2)		

[a]Khare and Shobha, Ref. 3.
[b]Khare and Gupta quoted in Ref. 1.

the Ochkur exchange amplitude. The results are represented by curve (3) in Fig. 1. Curve (1) in the same figure represents the values of DSC with MG direct and URG exchange amplitude. A comparison of these two curves shows that the Glauber approximation results agree better with experimental values than those with Ochkur approximation. As the energy of the incident electron increases the agreement of the results of Ochkur approximation with the experimental values improves but in no case is it superior to Glauber approximation.

The eikonal approximation results of Truhlar (see the curve designated by —...— of Fig. 2) are in poor agreement with the experimental results. In the table we present the calculated values of the integrated cross section at various energies with the MG approximation. They are in very good agreement with the experimental values of Van Wingarden.[1]

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