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Exchange correction to electron–hydrogen-molecule scattering cross section in the Glauber approximation

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The exchange correction to the differential scattering cross section for the electron–hydrogen-molecule scattering is derived. In the independent scattering center and Glauber approximation our expressions do not agree with those used in the published literature. The overall agreement between the calculated and the measured cross sections improves at higher angles and lower incident electron energies, where the exchange contribution is important.

I. INTRODUCTION

In the past decade electron-atom scattering has been studied extensively by various approximation methods,[1-6] depending on the energy range of the incident electron. On the other hand theoretical studies of electron-molecule scattering are not as extensive as for the atomic case. This is due to the complexity of the problem arising from the presence of many particles and the multicentered nature of the target with close-lying excited states.

The elastic scattering of electrons from the H_2 molecule was studied by Truhlar and Rice[7] in the intermediate-energy region using the Born and polarized Born approximation methods. The results obtained by these authors show reasonable trends when compared to the experimental values. However, the discrepancy between theoretical and experimental results is quite large. More recently Truhlar and co-workers[8,9] have applied rotational close coupling and body-frame close coupling with effective potentials to calculate electron scattering at intermediate energy of several molecules, and Dehmer and co-workers[10] have applied the multiple-scattering method. The Glauber[11] approximation leads to less expensive calculations, but it was quite successful when applied to the electron-H scattering, and it has been applied by Huang and Chan[12] to study the scattering of electrons from H_2. Unfortunately, their treatment of exchange scattering, as was pointed by Srivastava *et al.*,[13] contained some inaccuracies. Neither Ref. 12 nor Ref. 13 contain the detailed derivation of the final expressions used for the numerical evaluations. The exchange correction used was based on physical intuition.

The expressions of Refs. 12 and 13 are given below for comparison with the one obtained by us in a present paper:

$$\left(\frac{d\sigma}{d\Omega}\right)_{e^--H_2}=2(\tfrac{1}{4}|F+G|^2+\tfrac{3}{4}|F-G|^2)[1+j_0(qR)]\,, \tag{1}$$

$$\left(\frac{d\sigma}{d\Omega}\right)_{e^--H_2}=2[|F|^2+|G|^2+(|F|^2-|G|^2)j_0(qR)]\,. \tag{2}$$

Here, F and G are the atomic direct and exchange scattering amplitudes, q is the momentum transfer to the molecule, R is the internuclear separation, and j_0 is the spherical Bessel function of order zero.

In the present investigation we derive the expression for the exchange correction to the differential cross section for e^--H_2 scattering in the independent-atom model as it was used by Huang and Chan[12] and Srivastava *et al.*[13] Surprisingly, we found that the expressions for $(d\sigma/d\Omega)_{e^--H_2}$ in both Refs. 12 and 13 do not agree with ours. In order to compare the qualitative trend of this exchange correction with that found in Refs. 9 and 10 we have also calculated the e^--H_2 elastic scattering in Glauber approximation.

In the present paper the effects of a polarization potential have not been considered. A detailed study of the effects of such a potential on the differential cross section for e^--H_2 scattering was carried out by Truhlar and Brandt.[8]

The derivation of the differential cross section expressions for e^--H_2 scattering is presented in Sec. II. In Sec. III we present the numerical results of the present calculations and their discussion. Finally, Sec. IV contains the conclusions.

II. FORMULATION

The system consisting of the incident electron and the hydrogen molecule satisfies the Schrödinger equation

$$H\Psi = E\Psi \,, \tag{3}$$

where

$$H = \vec{p}_1^{\,2}/2m + H_m(2,3) + V_1(1,2,3) \,. \tag{4}$$

V_1 is the interaction energy of the incident electron 1, with momentum p_1, with the molecule, and H_m is the Hamiltonian of the molecule containing electrons 2 and 3. The H_2 wave function satisfies

$$H_m\psi = E_g\psi \,, \tag{5}$$

where E_g is the ground-state energy of the hydrogen molecule and ψ is the corresponding wave function. Using the antisymmetrized wave function Ψ and Eq. (5) in Eq. (3), one obtains readily the equation for the scattered wave ϕ as

$$\frac{\vec{p}_1^{\,2}}{2m}\phi(1) + \langle \psi(2,3) | V_1(1 - P_{12} - P_{13}) | \psi(2,3)\rangle \phi(1) = (E - E_g)\phi(1) \,. \tag{6}$$

In Eq. (6), P_{ij} is the space and spin exchange operator. The $\langle\,\rangle$ around the second term indicate an integration over space variables and sum over spin variables for electrons 2 and 3. In a straightforward manner we can calculate the scattering amplitude T as

$$\begin{aligned}\langle f | T | i\rangle = {} & \langle \phi_f(1)\psi_s(2,3) | V_1 | \phi_i(1)\psi_s(2,3)\rangle \\ & - \langle \phi_f(1)\psi_s(2,3) | V_1 P_{12}^s | \phi_i(1)\psi_s(2,3)\rangle \\ & \times \langle m_f\psi_\sigma(2,3) | P_{12}^\sigma | m_i\psi_\sigma(2,3)\rangle \\ & - \langle \phi_f(1)\psi(2,3) | V_1 P_{13}^s | \phi_i(1)\psi_s(2,3)\rangle \\ & \times \langle m_f\psi_\sigma(2,3) | P_{13}^\sigma | m_i\psi_\sigma(2,3)\rangle \,,\end{aligned} \tag{7}$$

where $|m\rangle$ is the electron spin state. The P's denote the exchange operators. The super or subscripts s and σ denote space and spin parts, respectively. On the right-hand side of Eq. (7), the first term denotes the electron-molecule direct scattering amplitude (f), while the space matrix elements of the other two terms are the exchange (g) scattering amplitude. From the spacial symmetry of the interaction potential V_1 and the wave function $\psi(2,3)$ for electrons 2 and 3, these two terms are identical. Now introducing the spin projection operator for the singlet spin state of electrons 2 and 3 and then using the definition of the differential scattering cross section as

$$\left(\frac{d\sigma}{d\Omega}\right)_{e^- - \mathrm{H}_2} = \tfrac{1}{2}\mathrm{Tr}(T^+T) \,, \tag{8}$$

we can easily obtain the well-known result[14] for the differential scattering cross section,

$$\left(\frac{d\sigma}{d\Omega}\right)_{e^- - \mathrm{H}_2} = |f - g|^2 \,. \tag{9}$$

We now express the molecular scattering amplitudes f and g in terms of atomic direct (F) and exchange (G) scattering amplitudes, respectively. For this purpose we take the spatial wave function of the hydrogen molecule in its ground $^1\Sigma_+$ state to be of the form

$$\psi_s(2,3) = \phi(2)\phi(3) \,, \tag{10}$$

where the orbital ϕ is a linear combination of atomic $1s$-state orbitals, one (u_1) centered at the origin and the other (u_2) centered at R, where R is the interatomic separation. As the hydrogen atomic orbital $u(r)$ is proportional to $e^{-\zeta r}$, the molecular wave function ψ_s is so chosen that it minimizes the expectation value

$$\frac{\langle \psi_s | H_m | \psi_s\rangle}{\langle \psi_s | \psi_s\rangle}$$

of H_m. The calculations are carried out for both $\zeta = 1.0$ (corresponding to an atomic-hydrogen orbital) and $\zeta = 1.2$, which is the value obtained[15] by the energy-minimization principle.

In solving Eq. (4), we use the fixed-center approximation and neglect the effect of the polarization potential, as mentioned earlier. Further, we assume that the radial matrix elements (RME) involving orbitals centered at the two different centers are related to RME at the same center by

$$\begin{aligned}\langle u_1 | v_1 | u_2\rangle & \approx Y\langle u_1 | v_1 | u_1\rangle \\ & = YV(r)\end{aligned}$$

and

$$\begin{aligned}\langle u_1 | v_2 | u_2\rangle & \approx Y\langle u_2 | v_2 | u_2\rangle \\ & = YV(\vec{r} - \vec{R}) \,,\end{aligned} \tag{11}$$

where Y is the overlap of the two orbitals. In Eq. (11),

$$v_1 = v(\vec{r}_1, \vec{r}_2) = -\frac{e^2}{|\vec{r}_1|} + \frac{e^2}{|\vec{r}_1 - \vec{r}_2|}$$

and $v_2 = v(\vec{r}_1 - \vec{R}, \vec{r}_2 - \vec{R})$. The solution ϕ_i then corresponds to the scattering solution due to the two-center potential v_1 and v_2. The potential $V(r)$ is the electron-hydrogen atom potential with u as hydrogen atomic orbital. To the extent that the contribution from double scattering can be neglected (this is valid for high-energy electron scattering where the de Broglie wavelength is smaller than the interatomic distance R), the molecular direct scattering amplitude f becomes

$$\begin{aligned}f = \langle \phi_f\psi_s(2,3) | V_1 | \phi_i\psi_s(2,3)\rangle & \approx (1 + e^{i\vec{q}\cdot\vec{R}})\langle \vec{k}_f | t | \vec{k}_i\rangle \\ & = (1 + e^{i\vec{q}\cdot\vec{R}})F \,,\end{aligned} \tag{12}$$

where t is the direct scattering amplitude due to hydrogenic atomic potential

$$V(r) = -\frac{e^2}{|\vec{r}|} + e^2\langle u_1|(\vec{r}-\vec{r}_1)^{-1}|u_1\rangle ,$$

and $\vec{q}$ $(=\vec{k}_f - \vec{k}_i)$ is the momentum transfer to the molecule. With the same approximations as above and using the orthogonality of bound and continuum orbitals, the molecular exchange scattering amplitude g can be obtained as

$$\begin{aligned} g &= (1+e^{i\vec{q}\cdot\vec{R}})\langle\vec{k}_f|t_{ex}|\vec{k}_i\rangle \\ &= (1+e^{i\vec{q}\cdot\vec{R}})G . \end{aligned} \tag{13}$$

Now substituting Eqs. (12) and (13) in Eq. (9) and averaging over rotational states of H_2, we finally obtain

$$\left(\frac{d\sigma}{d\Omega}\right)_{e^--H_2} = 2|F-G|^2[1+j_0(qR)] , \tag{14}$$

where j_0 is the spherical Bessel function of order zero. One can immediately see that this expression is different from Eqs. (1) and (2) used by Huang and Chan[12] and Srivastava *et al.*,[13] respectively.

III. NUMERICAL RESULTS

For numerical evaluation we use the expressions given by Huang and Chan[12] for direct and exchange atomic scattering amplitudes in Glauber approximation. For completeness we quote them below (atomic units are used):

$$F = \frac{2\pi\eta}{\sinh\pi\eta}\,\frac{1}{q^2}\left(\frac{q}{\lambda}\right)^{2i\eta}\left[(1+i\eta)\,{}_2F_1\!\left(1-i\eta,\ 1-i\eta;1;-\frac{\lambda^2}{q^2}\right)\right.$$
$$\left. +\,(1-i\eta)^2\frac{\lambda^2}{q^2}\,{}_2F_1\!\left(2-i\eta,\ 2-i\eta;2;-\frac{\lambda^2}{q^2}\right)\right]$$

and

$$G = \frac{2^{2-2i\eta}}{k_i^2}\,\Gamma(1-i\eta)\,\frac{-8+i\eta(4-q^2)}{(4+q^2)^{2-i\eta}} . \tag{15}$$

For elastic scattering

TABLE I. Differential scattering cross sections in units of a_0^2/sr for electrons from hydrogen molecules at the incident energy of 30 eV.

Angle (deg)	Experiment	Present calculation $\lambda=2.0$	Present calculation $\lambda=2.4$	Khare and Shobha (Ref. 16)
1		102.04	53.45	
2		75.82	43.20	
3		59.50	34.09	
4		49.2	28.77	
5		41.99	25.02	
6		36.59	22.19	
7		32.38	19.95	
8		28.97	18.14	
10		23.77	15.32	9.1
20	5.59	11.22	8.13	6.6
30	3.08	6.09	4.80	4.8
40	2.05	3.41	2.86	3.4
50	1.068	1.94	1.7	2.0
60	0.709	1.12	1.01	1.3
70	0.421	0.67	0.615	0.85
80	0.263	0.416	0.386	0.56
90	0.18	0.271	0.253	0.37
100	0.142	0.186	0.174	0.26
110	0.133	0.135	0.126	0.20
120	0.111	0.103	9.64×10^{-2}	0.15
130		8.34×10^{-2}	7.75×10^{-2}	
140		7.05×10^{-2}	6.55×10^{-2}	
150		6.21×10^{-2}	5.75×10^{-2}	
160		5.69×10^{-2}	5.26×10^{-2}	
170		5.41×10^{-2}	4.99×10^{-2}	
180		5.32×10^{-2}	4.91×10^{-2}	

$$q=2k_i\sin(\tfrac{1}{2}\theta),\quad \eta=1/v_i=1/k_i\,, \tag{16}$$

where k_i is the incident electron momentum. In these equations $\lambda=2\zeta$; thus we computed $d\sigma/d\Omega$ for the two values of $\lambda=2.0$ and 2.4.

For comparison with the results obtained from Eqs. (14)–(16), we have recalculated the values of $(d\sigma/d\Omega)_{e^--H_2}$ using Eqs. (1) and (2) with both values of λ. These values are not given in the present tables since Eqs. (1) and (2) are incorrect, but for 30-eV incident energy they are given for comparison in the figure. To indicate the effect of variation in λ on the results, we have presented results for both values in Tables I–IV.

To compare our results with those of the polarized Born approximation we have plotted in Fig. 1 the results of Khare and Shabha,[16] as given by Truhlar and Rice,[7] for the 30-eV incident electron energy. Besides these, the figure contains the experimental results of Williams[17] and Lloyd *et al.*[18] as normalized to the present calculations with $\lambda=2.4$ at 60°. From the figure, it is clear that the results of the present calculations are in better agreement with the experimental values as compared to those of Huang and Chan[12] and Srivastava *et al.*[13] This agreement is more at higher angles of scattering and lower energies. The normalization generally masks the comparison of theory to the experiment, as is evident from the figure.

To avoid this, we present in column 2 of the tables the unrenormalized values of the experiments. In Tables I and II, the last columns contain the results of the calculations of Khare and Shobha. Columns 3 and 4 contain the results of Glauber approximation for both the values of λ. Comparing the results of the Glauber and polarized Born approximations with the experimental values we notice that the Glauber results with the static potential alone are in better agreement with experiment than those of the polarized Born approximation. Further, comparing the results of column 4 of Tables I and II (corresponding to the value $\lambda=2.4$), with those in columns 3 (corresponding to the value $\lambda=2.0$) of all the tables, one can notice a definite improvement in the results of theory toward the experimental values, as expected. It is rather surprising to see the reasonable agreement of the results of Huang and Chan[12] with experiment, even though these authors have treated the exchange term inaccurately (see the Introduc-

TABLE II. Same as in Table I, but for 50-eV incident electron energy.

Angle (deg)	Experiment	Present calculation		Khare and Shobha (Ref. 16)
		$\lambda=2.0$	$\lambda=2.4$	
1		62.19	33.07	
2		44.41	24.87	
3		34.84	19.97	
4		28.85	16.87	
5		24.66	14.67	
6		21.51	13.01	
7		19.04	11.69	
8		17.04	10.61	
10		13.95	8.93	6.5
20	3.8	6.26	4.46	4.1
30	1.87	3.06	2.36	2.4
40	0.848	1.51	1.23	1.3
50	0.428	0.756	0.642	0.78
60	0.266	0.393	0.343	0.47
70	0.168	0.217	0.193	0.28
80	0.106	0.129	0.116	0.18
90	7.09×10^{-2}	8.29×10^{-2}	7.51×10^{-2}	0.14
100	5.87×10^{-2}	5.81×10^{-2}	5.28×10^{-2}	0.10
110	4.20×10^{-2}	4.39×10^{-2}	4.0×10^{-2}	0.07
120	3.84×10^{-2}	3.53×10^{-2}	3.23×10^{-2}	0.06
130		2.99×10^{-2}	2.73×10^{-2}	
140		2.64×10^{-2}	2.41×10^{-2}	
150		2.42×10^{-2}	2.20×10^{-2}	
160		2.27×10^{-2}	2.07×10^{-2}	
170		2.19×10^{-2}	2.0×10^{-2}	
180		2.16×10^{-2}	1.97×10^{-2}	

TABLE III. Same as in Table I, for an incident electron energy of 100 eV.

Angle (deg)	Experiment	Present calculation $\lambda = 2.0$	Present calculation $\lambda = 2.4$
1		30.49	16.45
2		21.44	11.96
3		16.96	9.65
4		14.16	8.19
5		12.18	7.15
6		10.67	6.35
7		9.48	5.71
8		8.49	5.18
10		6.93	4.32
20	1.803	2.77	1.92
30	0.795	1.09	0.826
40	0.417	0.431	0.349
50	0.159	0.182	0.155
60	9.00×10^{-2}	8.72×10^{-2}	7.69×10^{-2}
70	5.71×10^{-2}	4.93×10^{-2}	4.45×10^{-2}
80	3.47×10^{-2}	3.26×10^{-2}	2.99×10^{-2}
90	2.71×10^{-2}	2.41×10^{-2}	2.23×10^{-2}
100	2.38×10^{-2}	1.91×10^{-2}	1.78×10^{-2}
110	1.83×10^{-2}	1.57×10^{-2}	1.48×10^{-2}
120	1.59×10^{-2}	1.33×10^{-2}	1.25×10^{-2}
130		1.15×10^{-2}	1.09×10^{-2}
140		1.02×10^{-2}	9.65×10^{-3}
150		9.24×10^{-3}	8.76×10^{-3}
160		8.60×10^{-3}	8.16×10^{-3}
170		8.23×10^{-3}	7.81×10^{-3}
180		8.11×10^{-3}	7.70×10^{-3}

TABLE IV. Same as in Table II, for an incident electron energy of 200 eV.

Angle (deg)	Experiment	Present calculation $\lambda = 2.0$	Present calculation $\lambda = 2.4$
1		15.32	8.25
2		11.08	6.09
3		8.99	5.01
4		7.66	4.32
5		6.68	3.81
6		5.91	3.41
7		5.26	3.07
8		4.71	2.78
10		3.78	2.29
20	0.566	1.16	0.810
30	0.229	0.327	0.259
40	8.70×10^{-2}	10.4×10^{-2}	8.96×10^{-2}
50	4.19×10^{-2}	4.49×10^{-2}	4.05×10^{-2}
60	2.33×10^{-2}	2.61×10^{-2}	2.43×10^{-2}
70	1.71×10^{-2}	1.77×10^{-2}	1.68×10^{-2}
80	1.23×10^{-2}	1.25×10^{-2}	1.20×10^{-2}
90	8.98×10^{-3}	8.97×10^{-3}	8.66×10^{-3}
100	8.08×10^{-3}	6.45×10^{-3}	6.26×10^{-3}
110	5.13×10^{-3}	4.74×10^{-3}	4.61×10^{-3}
120		3.61×10^{-3}	3.52×10^{-3}
130		2.88×10^{-3}	2.81×10^{-3}
140		2.41×10^{-3}	2.36×10^{-3}
150		2.12×10^{-3}	2.08×10^{-3}
160		1.95×10^{-3}	1.91×10^{-3}
170		1.85×10^{-3}	1.82×10^{-3}
180		1.83×10^{-3}	1.79×10^{-3}

tion of Ref. 13). Both from the figure and the tables it is evident that the proper inclusion of the exchange term in Glauber formalism reduces the gap between the theory and experiment for the differential scattering cross section of electrons from hydrogen molecules.

IV. CONCLUSIONS

We have derived the exchange correction to the cross section for e^--H$_2$ molecule scattering within the independent-scattering-center approximation. This cross section has been expressed in terms of the atomic scattering amplitudes. The exchange contribution to $(d\sigma/d\Omega)_{e^- \text{-H}_2}$ derived in the present work differs from that used by the earlier investigators.[12,13] As in Refs. 12 and 13 the e^--H$_2$ scattering was treated in the Glauber approximation, and we used the same approximation both for direct and exchange e^--H atom scattering amplitudes. Our results are in better agreement with the experimental data than the polarized Born approximation results of Refs. 7 and 16. In the present calculations we used the improved treat-

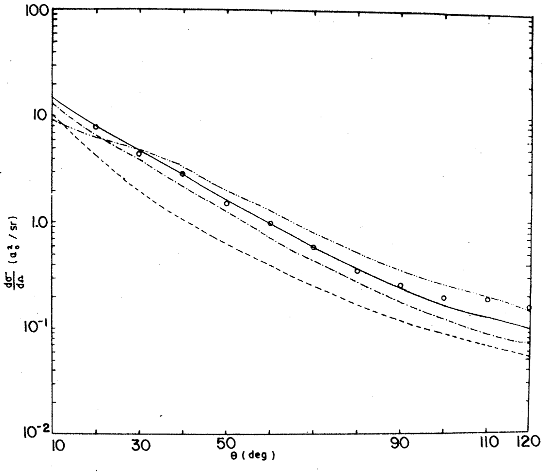

FIG. 1. Differential scattering cross section for e^--H_2 molecule elastic scattering with incident electron energy of 30 eV. The continuous line ——— corresponds to the present calculations; broken lines ---- indicate the results of Srivastava *et al.*[13]; a line and a dot -·-·-·-·-·-· indicate the results of Huang and Chan[12]; a line and two dots —··—··—··— indicate the results of Khare and Shobha[16]; and the open circle ○ indicates the experimental values of Williams[17] and Lloyd *et al.*[18]

ment of Khayrallah[19] for the exchange correction, and we found that the calculated cross sections agree well with experiment. The overall agreement improves at higher angles and low incident electron energies where the exchange contribution is important.

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