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Eikonal amplitude for electron-molecule collisions with effective complex potential: An application to H_2

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A tractable form of the Glauber eikonal amplitude for electron-molecule scattering is obtained with an effective complex potential. We report calculations of differential and integral cross sections for elastic scattering and pure rotational excitations, and of absorption cross sections (for sum of all electronic excitations and ionization processes) for e-H_2 collisions at 40—100 eV. The absorption potential is modeled following Valone, Thirumalai, and Truhlar. It is found that rotationally summed elastic cross sections (integral) are reduced by about (3—5)% when absorption is considered and total cross sections (including absorption cross sections) agree well with available experimental measurements.

I. INTRODUCTION

Recently, we have presented[1,2] a formulation of the Glauber eikonal scattering amplitude suitable for the study of electron- (positron-) molecule scattering at intermediate energies. In this method the scattering amplitude for a fixed molecular orientation is expanded in terms of a series in product of Bessel functions of increasing order. This amplitude is then utilized, in the framework of adiabatic approximation, in deriving the rotationally summed elastic and state-to-state rotational excitation cross sections. For electrons, we have made a systematic study of elastic scattering and rotational excitation cross sections of molecular targets hydrogen,[1-3] nitrogen,[4] and oxygen.[5] Computed cross sections are found to agree well with experimental observations and other theoretical results. For positron-hydrogen molecule scattering this method, interestingly, is found[6,7] to reproduce accurately experimental total cross sections below the threshold for positronium formation. In all these calculations we have considered the effective local electron- (positron-) molecule potential to be real. At intermediate energies, real electronic excitation of molecules is a dominant process and results in the loss of flux from the initial channel. A realistic effective local electron-molecule potential is necessarily complex in nature above the lowest inelastic threshold. The imaginary part of this complex potential, usually termed as absorption potential, takes into account the loss of flux from the initial channel. Considering this absorption part of electron-molecule potential we have derived in the present paper a tractable form of the Glauber eikonal scattering amplitude. Thus the effects of absorption on the rotationally summed elastic scattering and state-to-state rotational excitation cross sections for electron-molecule scattering can now be studied by using the Glauber approximation. Apart from these, contribution to total cross sections due to inelastic channels can be obtained by exploiting the optical theorem. As such the present Glauber amplitude might provide useful means for making a comparative study of electron and positron scattering at intermediate energies considering the effects of possible inelastic channels. The relevant expressions we have derived in the present paper are for molecular targets belonging to the point group $D_{\infty h}$, but similar expressions for molecules belonging to the point group $C_{\infty v}$ can readily be obtained.

For electron-atom scattering different absorption potentials[8-16] are now in use in the literature. Truhlar and co-workers have made a comparative study of a few of these in case of electron-helium[17] and electron-neon[18,19] scattering. Recently, Valone *et al.*[15] have shown that the absorption potential for electron-atom scattering can be obtained from the energy-dependent polarization potential. We have modeled the absorption potential for electron-molecule scattering following them and applied it to e-H_2 scattering at incident energies 40, 60, and 100 eV. Computed cross sections are compared with the available experimental obeservations.

II. SCATTERING AMPLITUDE AND CROSS SECTIONS

We consider the effective electron-molecule potential (local) or optical potential $V(\vec{r},\hat{R},E)$ describing the electron-molecule scattering to be complex:

$$V(\vec{r},\hat{R},E)=V_R(\vec{r},\hat{R},E)+iV_A(\vec{r},\hat{R},E)\ , \tag{1}$$

where $V_R(\vec{r},\hat{R},E)$, the real part of the potential, consists of the static potential $V_s(\vec{r},\hat{R})$, the effective local exchange potential $V_{\rm ex}(\vec{r},\hat{R}E)$, and the polarization potential $V_p(\vec{r},\hat{R},E)$:

$$V_R(\vec{r},\hat{R},E)=V_s(\vec{r},\hat{R})+V_{\rm ex}(\vec{r},\hat{R},E)+V_p(\vec{r},\hat{R},E)\ , \tag{2}$$

and $V_A(\vec{r},\hat{R},E)$ is the effective local absorption potential.

In case of a linear target potential (1) can be expanded in Legendre polynomials as

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$$V(\vec{r},\hat{R},E)=\sum_{\nu=0} V^{\nu}(r,E)P_{\nu}(\hat{r}\cdot\hat{R}) \ , \tag{3}$$

where

$$V^{\nu}(r,E)=V_R^{\nu}(r,E)+iV_A^{\nu}(r,E) \ ,$$

$$V_R^{\nu}(r,E)=V_s^{\nu}(r)+V_{\mathrm{ex}}^{\nu}(r,E)+V_p^{\nu}(r,E) \ .$$

In these expressions $\vec{r}$ is the position vector of the incident electron measured from the center of mass of the molecule, $\hat{R}$ is the unit vector along the internuclear axis $\vec{\mathrm{R}}$, and E is the impact energy. For molecules belonging to the point group $D_{\infty h}$ only the terms corresponding to even values of ν, including zero, survive in the expansion (3). We consider here terms with $\nu=0$ and 2 only.

With the use of potential (3) and the relation

$$\hat{r}\cdot\hat{R}=\cos\theta_r\cos\theta_m+\sin\theta_r\sin\theta_m\cos(\varphi_r-\varphi_m) \ ,$$

the Glauber eikonal scattering amplitude[2] for a fixed orientation of the molecular axis can be written as (we use atomic units throughout)

$$f(\theta,\hat{R})=-\frac{ik_i}{2\pi}\int e^{iqb\cos\varphi_r}(e^{-i\eta_R+\eta_A}-1)b\,db\,d\varphi_r \tag{4}$$

with

$$\eta_{R,A}=\chi_{R,A}(b,\theta_m)+\gamma_{R,A}(b,\theta_m)\cos[2(\varphi_r-\varphi_m)] \ ,$$

$$\begin{aligned}\chi_{R,A}(b,\theta_m)=&\frac{2}{v_i}\int_0^{\infty}V_{R,A}^0(r,E)dz\\ &+\frac{1}{v_i}(1-\tfrac{3}{2}\sin^2\theta_m)\\ &\times\int_0^{\infty}V_{R,A}^2(r,E)\frac{2z^2-b^2}{r^2}dz \ ,\end{aligned}$$

$$\gamma_{R,A}(b,\theta_m)=\tfrac{3}{2}\frac{\sin^2\theta_m}{v_i}\int_0^{\infty}V_{R,A}^2(r,E)\frac{b^2}{r^2}dz \ .$$

Here $\vec{\mathrm{b}}$ is the impact parameter vector defined as $\vec{\mathrm{r}}=\vec{\mathrm{b}}+\hat{k}_i z$, $m_e\vec{\mathrm{v}}_i=\hbar\vec{\mathrm{k}}_i$ is the momentum of the incident electron, $\vec{\mathrm{q}}=\hbar(\vec{\mathrm{k}}_i-\vec{\mathrm{k}}_f)$ is the momentum transfer to the molecule, and θ is the scattering angle. (θ_m,φ_m) defines the orientation of the molecular axis with respect to polar axis taken to be in the direction of $\vec{\mathrm{k}}_i$.

The φ_r integration in (4) is carried out by introducing a new variable $\Phi=\varphi_r-\varphi_m$ and expanding $\exp[iqb\cos(\Phi+\varphi_m)-i\gamma_R\cos(2\Phi)]$ in terms of Bessel functions J_n and $\exp[\gamma_A\cos(2\Phi)]$ in terms of modified Bessel function I_n. After some algebraic manipulation the amplitude (4) reduces to

$$f(\theta,\hat{R})=-ik_i\sum_{n=0} f_{2n}(\theta,\theta_m)\cos(2n\varphi_m) \ . \tag{5}$$

with

$$f_{2n}(\theta,\theta_m)=\begin{cases}\displaystyle\int J_0(qb)\left[C\sum_{p=0}(-i)^p\delta_p J_p(\gamma_R)I_p(\gamma_A)-1\right]b\,db & \text{for } n=0\\ \displaystyle\int CJ_{2n}(qb)\sum_{p=0}(-i)^{2n+p}\delta_p J_p(\gamma_R)[I_{p+n}(\gamma_A)+I_{p-n}(\gamma_A)]b\,db & \text{for } n\neq 0 \ .\end{cases}$$

$$C=\exp(-i\chi_R+\chi_A) \ ,$$

$$\delta_p=\begin{cases}1 & \text{for } p=0\\ 2 & \text{for } p\neq 0 \ .\end{cases}$$

This is the final expression for the Glauber eikonal amplitude for electron-molecule scattering when the molecular target is in a particular orientation and the scattering is described by the effective complex potential (3) with $\nu=0$ and 2. With the neglect of the imaginary part of the potential (3) we immediately regain the expression obtained earlier[2] by considering only the real part of it.

The above amplitude with a rigid rotor prescription for the molecular target yields, in the adiabatic approximation,[2,20,21] the differential scattering cross section (DCS) $I(J\rightarrow J',\ \theta)$ for the excitation process $J\rightarrow J'$ and the rotationally summed elastic DCS $\langle I(\theta)\rangle$:

$$I(J\rightarrow J',\ \theta)=\frac{k_i^2(2J'+1)}{16}\sum_{M=-J}^{J}\sum_{M'-J'}^{J'}\lambda_n^2\left|\left[\frac{(J-|M|)!}{(J+|M|)!}\frac{(J'-|M'|)!}{(J'+|M'|)!}\right]^{1/2}\times\int P_{J'}^{|M'|}(\cos\theta_m)f_{2n}(\theta,\theta_m)P_J^{|M|}(\cos\theta_m)\sin\theta_m d\theta_m\right|^2 \ , \tag{6}$$

with

$$2n=|M-M'|\ ,$$

$$\lambda_n=\begin{cases}2 & \text{for } n\neq 0\\ 1 & \text{for } n\neq 0\ ,\end{cases}\qquad (7)$$

$$\langle I(\theta)\rangle=\frac{k_i^2}{4}\sum_{n=0}\lambda_n\int|f_{2n}(\theta,\theta_m)|^2\sin\theta_m d\theta_m\ .$$

Equation (6) shows that the highest-order term in $f_{2n}(\theta,\theta_m)$ [Eq. (5)] determined by the maximum value of n that contributes to $I(J-J',\ \theta)$ depends upon the rotational states J and J'. For the transition $J=0\rightarrow J'=0$, for example, only the term with $n=0$ survives, while terms with $n\leq 2$ becomes effective for the transition $J=1\rightarrow J'=3$. It is found that $f_{2n}(\theta,\theta_m)$, for a particular value of n, converges when terms up to $p=4$ are considered [Eq. (5)]. The series in (7) converges rapidly with increasing n and truncation at $n=2$ gives well-convergent results for $\langle I(\theta)\rangle$ which does not depend upon the initial state J. Integrated state-to-state cross sections $\sigma(J\rightarrow J')$ or rotationally summed elastic cross sections $\langle\sigma_{\text{el}}\rangle$ can be computed using Eq. (6) or Eq. (7) in

$$\sigma=2\pi\int_0^\pi I(\theta)\sin\theta\, d\theta\ .\qquad (8)$$

According to optical theorem rotationally summed total cross sections $\langle\sigma_T\rangle$ is given by

$$\langle\sigma_T\rangle=\frac{4\pi}{k_i(2J+1)}\sum_{M=-J}^{J}F^I(JM\rightarrow JM,\ \theta=0)\ ,\qquad (9)$$

where F^I denotes the imaginary part of the amplitude F which is defined by the relation

$$F(JM\rightarrow J'M',\theta)=\int Y_{J'M'}^*(\hat{R})f(\theta,\hat{R})Y_{JM}(\hat{R})d\hat{R}\ .\qquad (10)$$

The expression (9) on simplification reduces to

$$\langle\sigma_T\rangle=-2\pi\int f_0^R(\theta=0,\theta_m)\sin\theta_m d\theta_m\ ,\qquad (11)$$

and becomes independent of the initial state J.

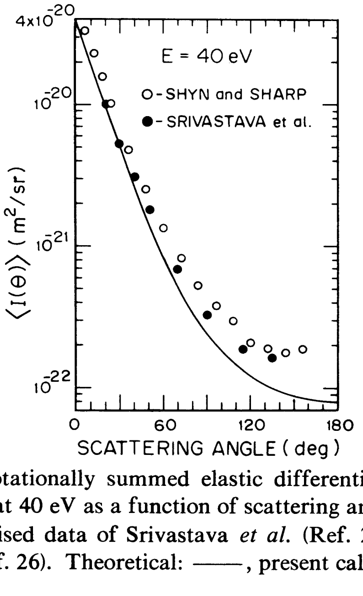

FIG. 1. Rotationally summed elastic differential scattering cross sections at 40 eV as a function of scattering angle. Experimental: ●, revised data of Srivastava *et al.* (Ref. 23); ○, Shyn and Sharp (Ref. 26). Theoretical: ——, present calculation.

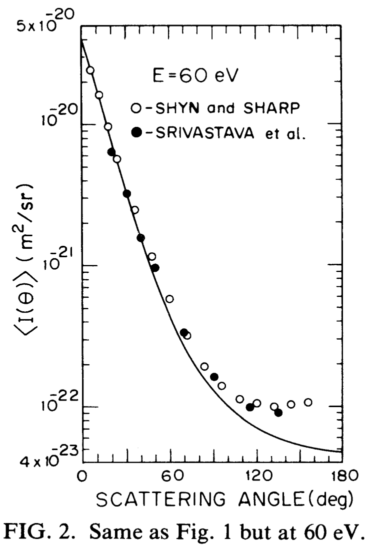

FIG. 2. Same as Fig. 1 but at 60 eV.

III. APPLICATION TO e-H_2 SCATTERING

A. Effective potential

In the present application to e-H_2 scattering the following simple effective potential is considered. First, for the real part of the potential (3) we have neglected exchange and the energy dependence of the polarization potential. The real potential is taken to be potential model B (without exchange) of Bhattacharyya *et al.*[3] so that a direct comparison of the present cross sections with those obtained earlier[3] neglecting absorption can be made to ascertain the effects of absorption on state-to-state and elastic scattering cross sections. Second, the absorption potentials $V_A^\nu(r,E)$ are modeled following Valone *et al.*:[15]

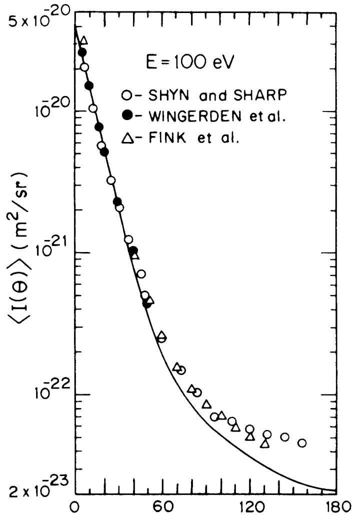

FIG. 3. Rotationally summed elastic differential scattering cross sections at 100 eV as a function of scattering angle. Experimental: ○, Shyn and Sharp (Ref. 26); ●, Wingerden *et al.* (Ref. 25); △, Fink *et al.* (Ref. 24), the data at 10° and 20° coincide with those of Wingerden *et al.* Theoretical: ——, present calculation.

TABLE I. Comparison of rotationally summed elastic DCS $\langle I(\theta)\rangle$ (in 10^{-21} m^2/sr) with and without absorption for e-H_2 scattering.

	With absorption			Without absorption[a]		
	E (eV)			E (eV)		
θ (deg)	40	60	100	40	60	100
0	38.24	40.39	42.03	36.06	38.02	39.71
5	28.42	27.88	25.81	26.99	26.63	25.02
10	20.24	18.48	15.35	19.62	18.12	15.28
15	14.39	12.26	9.138	14.26	12.30	9.279
20	10.24	8.137	5.424	10.36	8.334	5.605
25	7.290	5.404	3.225	7.524	5.643	3.388
30	5.201	3.600	1.940	5.473	3.830	2.070
35	3.724	2.417	1.193	3.994	2.618	1.291
40	2.685	1.644	0.759	2.934	1.812	0.831
50	1.441	0.809	0.348	1.632	0.918	0.385
60	0.825	0.442	0.189	0.962	0.510	0.208
70	0.509	0.269	0.118	0.606	0.311	0.130
80	0.340	0.180	0.084	0.409	0.207	0.091
90	0.244	0.130	0.065	0.293	0.149	0.070
100	0.185	0.101	0.052	0.222	0.115	0.057
110	0.148	0.083	0.044	0.176	0.094	0.047
120	0.124	0.071	0.037	0.146	0.080	0.040
130	0.107	0.063	0.032	0.126	0.071	0.034
140	0.096	0.057	0.028	0.113	0.064	0.030
150	0.088	0.053	0.025	0.104	0.064	0.027
160	0.084	0.051	0.023	0.098	0.057	0.025
170	0.081	0.049	0.022	0.094	0.055	0.023
180	0.080	0.047	0.021	0.093	0.054	0.023

[a] Reference 3 (model B, without exchange). Cross sections at 60 eV are obtained in the present work.

$$V_A^v(r,E)=\frac{V_p^v(r,E)(E-\epsilon_1)^{1/2}}{[\epsilon_1+U(r)]^{1/2}}\ , \qquad (12)$$

with

$$V_p^v(r,E)=V_p^v(r)/[1+E/U(r)]\ ,$$

$$U(r)=\omega^2r^2/12\ ,$$

where ϵ_1 is the lowest electronic excitation energy of the target and ω is the average excitation energy. Energy dependence of the polarization potential as shown above is for atomic targets. For molecular targets it should be somewhat different which might be taken into account by treating ω as an adjustable parameter. However, we have taken $\omega=0.564$ a.u., the ionization energy of H_2 and $\epsilon_1=0.4178$ a.u. the threshold for the excited state $B\,^1\Sigma_u^+$ of H_2. The adiabatic polarization potential determined by Henry and Lane,[22] which is used in real part of the potential (model B), is considered for $V_p^v(r)$. The absorption potential so defined would account for the real electronic excitation and ionization processes of H_2.

TABLE II. Comparison of different integral cross sections (in 10^{-20} m^2) with and without absorption for e-H_2 scattering.

E (eV)	$\sigma(0\rightarrow0)$	$\sigma(0\rightarrow2)$	$\sigma(1\rightarrow1)$	$\sigma(1\rightarrow3)$	$\langle\sigma_{el}\rangle$	$\langle\sigma_{el}\rangle^a$
40	1.576	0.115	1.622	0.070	1.694	1.66[b]
	1.648[c]	0.130[c]	1.700[c]	0.079[c]	1.780[c]	2.50[d]
60	1.139	0.107	1.182	0.065	1.248	1.26[b]
	1.179[c]	0.118[c]	1.226[c]	0.071[c]	1.299[c]	1.27[d]
100	0.731	0.086	0.766	0.052	0.818	0.77[d]
	0.748[c]	0.092[c]	0.785[c]	0.056[c]	0.841[c]	0.88[e]

[a] Experimental.

[b] Srivastava *et al.* (Ref. 23). These data will be slightly changed if He data of Register *et al.* (Ref. 27) are used to regain H_2 data.

[c] Without absorption (model B, without exchange, Ref. 3; cross sections at 60 eV are obtained in the present work).

[d] Shyn and Sharp (Ref. 26).

[e] Wingerden *et al.* (Ref. 25).

B. Results and discussions

We have computed state-to-state and average elastic scattering cross sections, both differential and integral, at impact energies 40, 60, and 100 eV. Total cross sections at these energies are also obtained by using the optical theorem. Numerical procedures for computing these cross sections are described elsewhere[4] in detail.

In Figs. 1–3 we have compared the average elastic DCS $\langle I(\theta)\rangle$ with a few recent experimental measurements[23–26] at relevant energies. The experimental data of Srivastava *et al.*[23] shown are obtained from their measured ratios of H_2 and He cross sections and the absolute He cross sections of Register *et al.*[27] At 40 eV (Fig. 1) the present cross sections reproduce well the angular dependence of experimental data of Shyn and Sharp[26] at small scattering angles, but are somewhat smaller in magnitude. The revised[23,27] data of Srivastava and co-workers are in good agreement at small angles. At 60 eV (Fig. 2) the agreement with both these measurements becomes better both in magnitude and angular dependence. At 100 eV (Fig. 3) the experimental data of Shyn and Sharp, van Wingerden *et al.*,[25] and Fink *et al.*[24] are well reproduced over a considerable angular region. At all energies considered here maximum deviation from the measured data, which reduces with increasing energy, are found to occur at large scattering angles.

In Table I we have presented cross sections $\langle I(\theta)\rangle$ with and without absorption for comparison. Cross sections without absorption at 40 and 100 eV are reported earlier by Bhattacharyya *et al.*[3] (model *B*, without exchange), while those at 60 eV are from the present work. It is found that cross sections show sharper rise at small scattering angles when absorption potential is taken into consideration, but they decrease for most part of the scattering angles. The angular region where cross sections are found to increase shortens with increasing energy. Rotational excitation DCS $I(J\rightarrow J+2)$ are also affected to some extent by the inclusion of absorption potential (not shown).

In Table II integral cross sections $\sigma(J\rightarrow J')$ and $\langle\sigma_{\rm el}\rangle$ with and without absorption are compiled. $\langle\sigma_{\rm el}\rangle$ determined experimentally by different workers[23,25,26] are also included in it for comparison. It is observed that the effects of absorption on $\langle I(\theta)\rangle$ (Table I) are reflected on the corresponding cross sections $\langle\sigma_{\rm el}\rangle$. When absorption potential is included $\langle\sigma_{\rm el}\rangle$ is reduced by about 4.8% at 40 eV and 2.7% at 100 eV. At any energy, effects of absorption are strongest for rotationally inelastic cross sections $\sigma(J\rightarrow J+2)$ (for instance at 40 eV, both the pure elastic cross sections are diminished by 5%, but the inelastic ones are diminished by 11%). Present $\langle\sigma_{\rm el}\rangle$ cross sections are in good agreement with those obtained experimentally by different workers.[23,25,26] The only exception is the measurements of Shyn and Sharp[26] at 40 eV which is somewhat higher in magnitude.

TABLE III. Total and absorption cross sections (in 10^{-20} m^2) for e-H_2 scattering.

E (eV)	$\langle\sigma_T\rangle^{\rm a}$	$\langle\sigma_{\rm abs}\rangle^{\rm a}$	$\langle\sigma_T\rangle^{\rm b}$
40	3.28	1.59	3.98$^{\rm c}$
			4.30$^{\rm d}$
			4.06$^{\rm e}$
60	2.55	1.30	3.34$^{\rm c}$
			3.20$^{\rm e}$
100	1.77	0.95	2.51$^{\rm c}$
			2.56$^{\rm d}$
			2.44$^{\rm e}$

[a] Present calculations.
[b] Experimental.
[c] Wingerden *et al.* (Ref. 28).
[d] Hoffman *et al.* (Ref. 29).
[e] Deuring *et al.* (Ref. 30).

Total cross sections $\langle\sigma_T\rangle$ obtained through optical theorem and absorption cross sections $\langle\sigma_{\rm abs}\rangle=\langle\sigma_T\rangle-\langle\sigma_{\rm el}\rangle$ are given in Table III. Total cross sections measured by van Wingerden *et al.*,[28] Hoffman *et al.*,[29] and Deuring *et al.*[30] are also presented in it. It is observed that computed $\langle\sigma_T\rangle$ at each energy underestimates all three measurements. Best agreement however is found to occur with the measurements of Deuring *et al.* As the impact energy E increases disagreement between theoretical and measured $\langle\sigma_T\rangle$ increases. This is because the present absorption potential yields $\langle\sigma_{\rm abs}\rangle$ which decreases at a faster rate with increasing energy.

IV. CONCLUSIONS

In the present paper we have derived the Glauber eikonal amplitude for electron-molecule scattering for an effective local complex potential. An application to e-H_2 scattering with a simple absorption potential yields reasonably accurate total cross sections. More realistic absorption potential and inclusion of exchange might yield better cross sections. Absorption potential is found to reduce the integral elastic scattering cross sections. In terms of state-to-state integral cross sections the pure rotational excitation cross sections are affected most compared to pure elastic cross sections.

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