

Ab initio inclusion of polarization effects in the Schwinger multichannel formulation: Application to elastic e -H₂ scattering

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To assess the accuracy with which polarization is represented in the Schwinger multichannel formulation, we have calculated elastic integral and differential scattering cross sections for e -H₂ collisions from 1 to 10 eV. Our *ab initio* results are found to be in good agreement with other recent theoretical studies and with a variety of experimental data including measured differential cross sections. Our method is designed to be applicable to electronically inelastic collisions and to closed-shell target molecules of arbitrary geometry.

I. INTRODUCTION

Polarization effects are known to be very important¹ for low-energy electron collisions with molecules which do not possess large permanent dipole moments. In these cases the polarization interaction has a significant effect on the overall shape and magnitude of the scattering cross section as well as on the width and position of resonances. Hence, there is considerable need for computationally feasible methods which can reliably include these effects. Although substantial progress has been made for some systems (most notably H₂ and N₂), no single method has yet been demonstrated for general use, i.e., for elastic and electronically inelastic collisions with both linear and non-linear molecular targets.

We begin by briefly reviewing some of the commonly used approaches for including polarization effects. These effects arise from the distortion of the molecular charge distribution by the electric field of the incident electron. In the adiabatic approximation,^{2,3} the polarization potential for a particular value of \vec{r} is calculated by allowing the molecular orbitals to fully relax in the presence of a negative charge *fixed* at \vec{r} . However, this approximation fails in the near vicinity of the molecule where nonadiabatic or dynamic corrections⁴⁻⁶ become important. A widely used and semiempirical approach to these dynamical effects assumes the known asymptotic form¹ of the polarization potential and includes a parameter-dependent cutoff function to mimic the nonadiabatic corrections. This method is easy to implement, but more complete treatments^{2,3} have revealed some of its inherent inadequacies. A further drawback is the need for parameters which are usually obtained by "tuning" so as to reproduce known features in the cross sections. This last difficulty is avoided in the polarized orbital method⁴⁻⁹ where Temkin's criterion¹⁰ is used to include nonadiabatic effects in an approximate but parameter-free fashion. However, the utility of the polarized orbital approach depends considerably on the particular way in which the method is implemented.⁶ Recently, another parameter-free model of polarization¹¹ has been applied to elastic scattering by H₂ and N₂. This model used the free-electron-gas correlation

energy to represent polarization effects¹² in the near vicinity of the molecule and the known asymptotic form to represent long-range polarization effects. Comparison of the results obtained by this approach with those of more elaborate studies indicates that this method overestimates polarization effects somewhat.

Polarization effects arise from virtual electronic excitation of the target and can be represented by the inclusion of energetically closed channels in the expansion of the scattering wave function. Such an expansion in actual target eigenstates can converge slowly. Expansions in pseudostates generally converge faster and hence these pseudostates are often used both in close-coupling expansions¹³ or in the optical potentials which represent the polarization effects.^{14,15} Although these methods have a firmer theoretical basis than those described above, their application generally requires considerably greater effort. These pseudostates are also known to lead to nonphysical or spurious resonances in the scattering cross section. The number of such spurious resonances increases with the number of pseudostates although the resonance widths become narrower. Techniques for smoothing the T matrices across these resonances have been proposed.¹⁶

In two recent papers^{17,18} we have detailed the formal development of a Schwinger multichannel (SMC) theory for use in electron-molecule scattering and its first application to electronically inelastic e -H₂ collisions. In these applications we neglected the contribution from closed channels for consistency in comparing with the results of previous theoretical studies. However, the formulation also allows for the inclusion of a substantial number of closed electronic channels to represent polarization effects¹⁹ and, due to the manner in which the open- and closed-channel spaces are coupled, the SMC formulation is free of spurious singularities on the real energy axis above the inelastic threshold. Further, as implemented, our method is designed to be applicable to closed-shell target molecules of arbitrary geometry.

In the present paper we report results obtained with this method for elastic e -H₂ scattering including closed-channel effects. This system provides a good test of how effectively the formulation can represent the effects of po-

larization since accurate experimental and theoretical cross sections are available for comparison. A brief review of our theoretical formulation is provided in Sec. II. The computational details of our study can be found in Sec. III together with a discussion of our results and a comparison with other studies. In Sec. IV we summarize our results and conclusions.

II. THEORY

The details of the SMC formulation have been discussed previously¹⁷⁻¹⁹ and hence we give only a brief review here. Our method begins with the projected Lippman-Schwinger equation

$$P\Psi_n^{(+)} = \frac{1}{\sqrt{N+1}} S_n + G_p^{(+)} V \Psi_n^{(+)}, \quad (2.1)$$

where $\Psi_n^{(+)}$ is the total $(N+1)$ -particle wave function with plane-wave and outgoing-wave boundary conditions for the n th channel. The projection operator P defines the open-channel space in terms of the N -particle eigenfunctions of the target Hamiltonian H_N :

$$P = \sum_{m=1}^{N_0} |\Phi_m(1,2,\dots,N)\rangle \langle \Phi_m(1,2,\dots,N)| \quad (2.2)$$

and

$$H_N |\Phi_m\rangle = E_m |\Phi_m\rangle, \quad E - E_m > 0 \quad (2.3)$$

where E is the total energy of the $(N+1)$ -particle system. In Eq. (2.1), S_n is the free-particle solution of the unperturbed Hamiltonian $H_0 = H_N + T_{N+1}$ and is given by

$$S_n = \Phi_n e^{i\vec{k}_n \cdot \vec{r}_{N+1}}. \quad (2.4)$$

The interaction between the incident electron and the target is

$$V = H_{N+1} - H_0 = \sum_{i=1}^N \frac{1}{|\vec{r}_i - \vec{r}_{N+1}|} - \sum_{\alpha} \frac{Z_{\alpha}}{|\vec{R}_{\alpha} - \vec{r}_{N+1}|}. \quad (2.5)$$

The outgoing-wave Green's function $G_p^{(+)}$ defined in the open-channel space can be written as

$$G_p^{(+)} = \sum_{m=1}^{N_0} |\Phi_m\rangle g_m^{(+)}(\vec{r}_{N+1}, \vec{r}'_{N+1}) \langle \Phi_m| \quad (2.6)$$

with

$$g_m^{(+)}(\vec{r}, \vec{r}') = -\frac{1}{2\pi} \frac{e^{ik_m |\vec{r} - \vec{r}'|}}{|\vec{r} - \vec{r}'|}. \quad (2.7)$$

To define a complete equation for $\Psi_n^{(+)}$ we must recover the unprojected component of Eq. (2.1). This is accomplished via the projected Schrödinger equation

$$[\hat{H} - a(P\hat{H} + \hat{H}P)]\Psi_n^{(+)} = a(VP - PV)\Psi_n^{(+)}, \quad (2.8)$$

where $\hat{H} = E - H_{N+1}$ and a is an arbitrary parameter. The above equation contains information about the closed channels without defining the closed-channel Green's function which would require the inclusion of target continuum states.²⁰ As shown by Takatsuka and McKoy,^{17,19} a simple combination of Eqs. (2.1) and (2.8) together with $a = (N+1)/2$ defines a complete equation for $\Psi_n^{(+)}$, viz.,

$$\left[\frac{1}{2}(PV + VP) - VG_p^{(+)}V + \frac{1}{N+1} \left[\hat{H} - \frac{N+1}{2}(P\hat{H} + \hat{H}P) \right] \right] \Psi_n^{(+)} = \frac{1}{\sqrt{N+1}} VS_n. \quad (2.9)$$

Based on Eq. (2.9), a variational functional for the fixed-nuclei scattering amplitude is

$$f^B(\vec{k}_m, \vec{k}_n) = -\frac{1}{2\pi} \frac{\langle S_m | V | \Psi_n^{(+)} \rangle \langle \Psi_m^{(-)} | V | S_n \rangle}{\left\langle \Psi_m^{(-)} \left| \left[\frac{1}{2}(PV + VP) - VG_p^{(+)}V + \frac{1}{N+1} \left[\hat{H} - \frac{N+1}{2}(P\hat{H} + \hat{H}P) \right] \right] \right| \Psi_n^{(+)} \right\rangle}, \quad (2.10)$$

where the superscript B on f^B indicates that this quantity is calculated in the body-fixed (molecular) reference frame.¹

In our procedure $\Psi_n^{(+)}$ is expanded in a basis of $(N+1)$ -particle Slater determinants which are constructed from an orthogonal set of molecular orbitals, additional basis functions, and plane-wave functions, if necessary. However, unlike the Feshbach partitioning technique,²¹ we make no distinction among the open and closed configurations in $\Psi_n^{(+)}$. The molecular orbitals and additional basis functions used to construct the Slater determinants are further expanded in Cartesian Gaussian functions. With this choice of basis, all of the matrix elements appearing in Eq. (2.1), except for the matrix elements of $VG_p^{(+)}V$, can be evaluated analytically for molecules of

arbitrary geometry. However, by inserting an approximate closure relation around $G_p^{(+)}$ (see Ref. 18), these matrix elements can also be obtained in closed form.²²⁻²⁴ This insertion basis also consists of Cartesian Gaussian functions, but it can be larger than the set used to expand $\Psi_n^{(+)}$. A criterion for the completeness of the insertion basis can be obtained by observing how the scattering matrix approaches unitarity.

This formulation allows us to calculate an analytic approximation to the body-frame fixed-nuclei^{1,25} scattering amplitude for molecules of arbitrary geometry. As discussed in our previous paper,¹⁸ we then expand $f^B(\vec{k}_m, \vec{k}_n)$ in a partial-wave series and make the requisite transformation into the laboratory frame. After accounting for the random orientation of the target, the physical

TABLE I. Basis set for these calculations.^a

SCF ^b		${}^2\Sigma_{g,u}^+$ ^c	${}^2\Pi_{g,u}$ ^d	Extra insertion ^e	
$A=(0,0,\pm 0.7)$					
$l m n$	α		$l m n$	α	$l m n$
0 0 0	33.6444		1 0 0	1.08	0 0 0
0 0 0	5.05796		1 0 0	0.54	0 0 0
0 0 0	1.1468 ^f		1 0 0	0.18	0 0 0
0 0 0	0.321144		1 0 0	0.06	0 0 1
0 0 0	0.101309		1 0 0	0.02	0 0 1
0 0 0	0.03		1 0 0	0.01	1 0 0
0 0 1	1.1142				1 0 0
0 0 1	0.2592				
0 0 1	0.06				
$A=(0,0,0)$					
		$l m n$	α		$l m n$
		0 0 0	0.01		0 0 0
		0 0 1	0.005		0 0 1
		0 0 2	0.4		0 0 1
		0 0 2	0.1		0 0 2
		0 0 2	0.025		0 0 2
					0 0 2

^aCartesian Gaussian functions defined by $X_{lmn}(\alpha) = N_{lmn}(x - A_x)^l(y - A_y)^m(z - A_z)^n e^{-\alpha|r - \vec{A}|^2}$.

^bBasis set used for the $X^1\Sigma_g^+(1\sigma_g)^2$ state of H_2 .

^cAdditional functions for the expansion of the scattering functions of ${}^2\Sigma_{g,u}^+$ symmetries.

^dSame as c but for ${}^2\Pi_{g,u}$ symmetries.

^eAdditional functions used in the insertion around $VG_p^{(+)}V$.

^fThe first three basis functions are contracted with coefficients of 0.025374, 0.189683, and 0.85293, respectively.

differential cross section is obtained in the usual manner by performing the appropriate average-over-initial and sum-over-final spin states.

III. PROCEDURES AND RESULTS

To assess the effectiveness with which closed-channel effects can be represented in our method, we have calcu-

lated elastic integral and differential cross sections for $e-H_2$ scattering from 1 to 10 eV. This constitutes a non-trivial test of our theory since the exact static-plus-exchange (ESE) integral cross sections are known to be

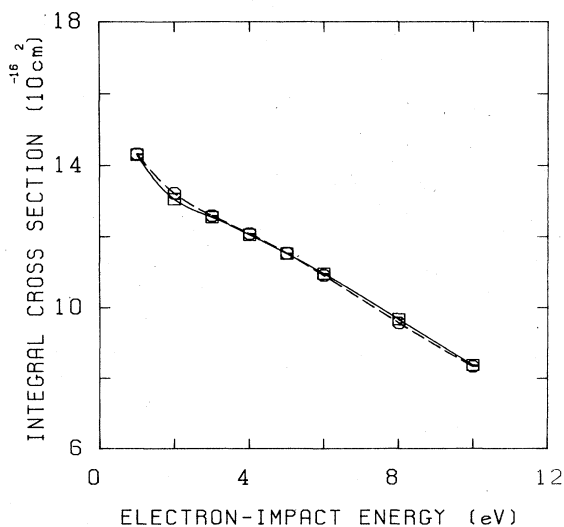


FIG. 1. Elastic cross sections for $e-H_2$ scattering in the static-exchange (SE) approximation: present results (\square), ESE results of Ref. 28 (\circ).

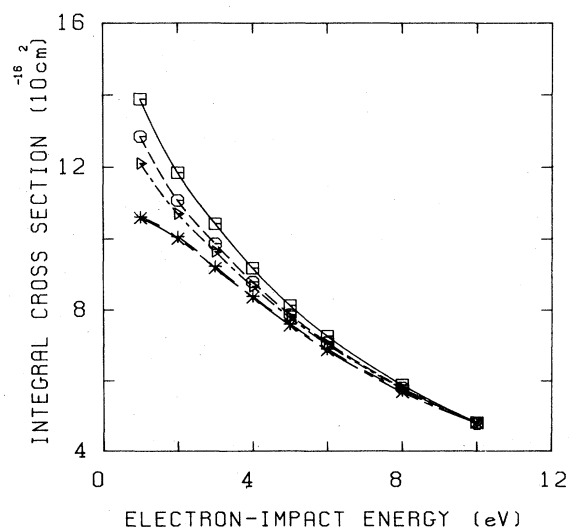


FIG. 2. Elastic cross sections for the ${}^2\Sigma_g$ symmetry: present SE results (\square), present results including only singlet-coupled pseudostates in the closed-channel expansion (\circ), present results including singlet-coupled and triplet-coupled pseudostates (\triangle), static-plus-exchange-plus-polarization (SEP) results of Ref. 15 (\times), SEP results of Ref. 6 ($+$).

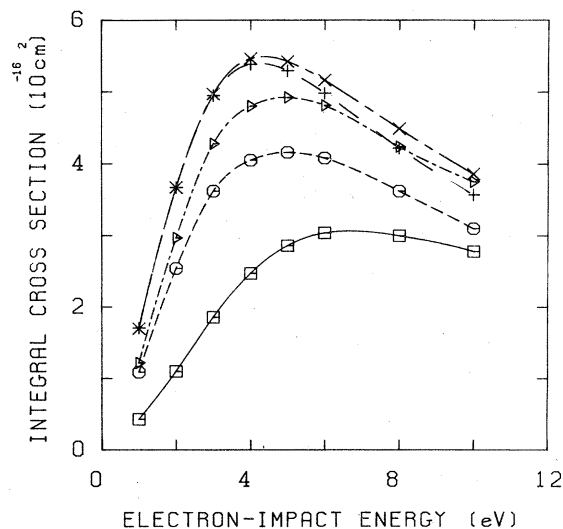


FIG. 3. Elastic cross sections for the $2^2\Sigma_u$ symmetry: same labels as in Fig. 2.

quite different from measured values in this energy range (cf. Fig. 5). Further, the $e\text{-H}_2$ system has been extensively studied and accurate experimental²⁶ and theoretical^{6,15} results for elastic scattering are available.

Our calculations are performed within the framework of the fixed-nuclei approximation.^{1,25} Here, the nuclei are held fixed at their equilibrium values and the dependence of the scattering amplitude on internuclear separation is neglected. The rotational levels are treated as degenerate and the physical cross sections are obtained by averaging the fixed-nuclei results over all molecular orientations. Unless otherwise stated, atomic units are used throughout.

For the ground state of H_2 we used a self-consistent-field (SCF) wave function obtained with a $[6s\ 3p/4s\ 3p]$ Cartesian Gaussian basis at an internuclear separation of

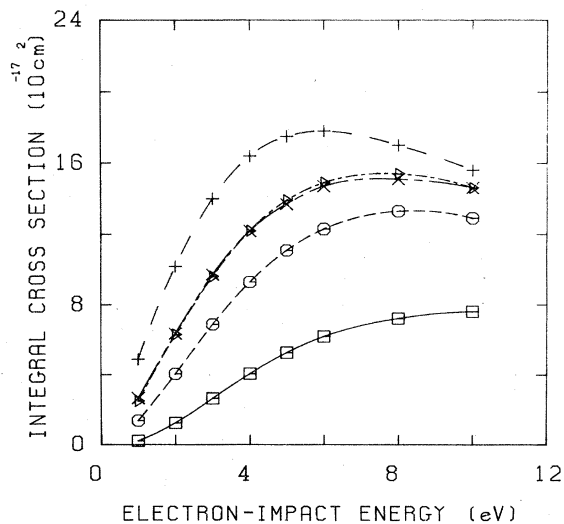


FIG. 4. Elastic cross sections for the $2^2\Pi_u$ symmetry: same labels as in Fig. 2.

TABLE II. Integral elastic cross sections for $e\text{-H}_2$ (10^{-16} cm^2).

Impact energy (eV)	JB ^a	GM ^b	SC ^c	SMC ^d
1	13.1	12.84	12.48	13.59
2	15.4	14.80	14.51	14.32
3	16.2	15.65	15.14	14.92
4	15.7	15.49	15.03	14.71
5	14.9	14.74	14.36	14.13
6	13.9	13.77	13.48	13.39
8	12.0	11.79	11.68	11.64
10	10.3	10.09	10.11	10.11

^aExperimental results of Ref. 29.

^bCalculated results of Ref. 6.

^cInterpolated from the results of Ref. 15.

^dPresent results.

$1.4a_0$. The exponents and contraction coefficients are from the $[5s\ 2p/3s\ 2p]$ set given by Huzinaga²⁷ together with an additional set of diffuse s - and p -type functions. For convenience, the exponents and contraction coefficients are given in Table I. With this basis we obtain a SCF energy of $-1.13295E_h$ and values of $\alpha_1=4.54a_0^3$, $\alpha_{||}=6.53a_0^3$ for the perpendicular and parallel components of the polarizability, respectively. These polarizabilities are obtained from a SCF finite-field calculation and can be compared to the accurate values of $\alpha_1=4.58a_0^3$, $\alpha_{||}=6.39a_0^3$. A set of H_2^- orbitals calculated with the same SCF basis was Schmidt orthogonalized to the occupied $1\sigma_g$ orbital and the resulting pseudoorbitals used to construct the $(N+1)$ -particle determinants in the expansion of Ψ_1^{\pm} . The use of these one-particle pseudoorbitals reduces the number of terms needed in the expansion of the closed-channel space compared to the number required if the regular SCF virtual orbitals are used. The Gaussian basis sets used as additional scattering functions

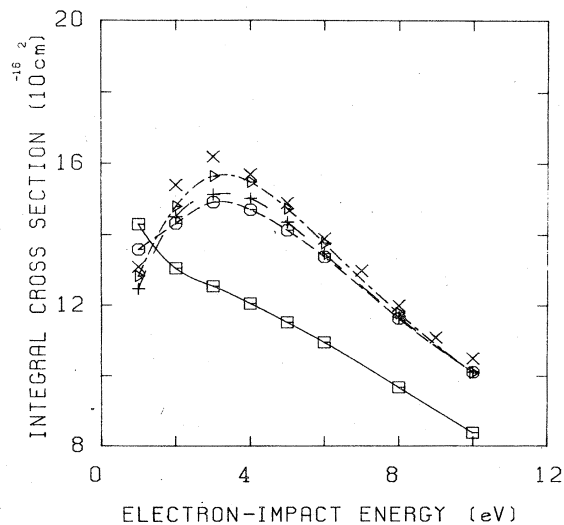


FIG. 5. Elastic cross sections for $e\text{-H}_2$ scattering: present SE results (\square), present SEP results (\circ), SEP results of Ref. 15 ($+$), SEP results of Ref. 6 (\triangle), experimental results of Ref. 29 (\times).

TABLE III. Differential cross sections for elastic $e\text{-H}_2$ collisions (10^{-16} cm^2).

Scattering angle (deg)	Impact energy (eV)							
	1	2	3	4	5	6	8	10
0	0.409	0.769	1.42	1.92	2.25	2.44	2.50	2.43
10	0.414	0.760	1.39	1.89	2.20	2.39	2.45	2.38
20	0.430	0.735	1.32	1.77	2.07	2.24	2.30	2.23
30	0.458	0.703	1.21	1.61	1.86	2.01	2.06	1.99
40	0.504	0.676	1.09	1.41	1.62	1.74	1.78	1.70
50	0.570	0.667	0.973	1.21	1.37	1.46	1.47	1.39
60	0.657	0.688	0.890	1.05	1.14	1.19	1.17	1.09
70	0.767	0.747	0.852	0.927	0.964	0.972	0.917	0.830
80	0.896	0.846	0.868	0.867	0.848	0.817	0.727	0.635
90	1.04	0.983	0.936	0.868	0.797	0.730	0.605	0.506
100	1.19	1.15	1.05	0.922	0.805	0.704	0.544	0.433
110	1.34	1.33	1.19	1.02	0.859	0.725	0.526	0.398
120	1.49	1.51	1.36	1.14	0.941	0.775	0.533	0.383
130	1.61	1.69	1.52	1.27	1.03	0.838	0.550	0.373
140	1.72	1.84	1.67	1.39	1.13	0.900	0.567	0.363
150	1.81	1.97	1.80	1.50	1.21	0.953	0.579	0.351
160	1.87	2.06	1.89	1.58	1.27	0.993	0.586	0.342
170	1.90	2.11	1.95	1.63	1.31	1.02	0.589	0.335
180	1.92	2.13	1.98	1.65	1.32	1.03	0.591	0.333

and in the insertion basis are also shown in Table I. For the energies considered here, expansion of the scattering functions solely in a discrete basis should be adequate. Also, for the purpose of this study we restrict the partial wave expansion of the scattering amplitude (see Sec. II) to values of $l \leq 3$.

In the body frame all calculated results include contributions from the ${}^2\Sigma_g$, ${}^2\Sigma_u$, ${}^2\Pi_u$, and ${}^2\Pi_g$ symmetries in $\Psi_1^{(\pm)}$. Of the available scattering basis, no more than 18 (12) spatial functions were used to construct the open-channel determinants in the expansion of $\Psi_1^{(\pm)}$ for Σ (Π) symmetries. For the Σ symmetries the scattering set consists of a mixture of pseudoorbitals and additional functions chosen to improve the flexibility of the basis. However, since there are no π orbitals in the pseudoorbital set, the scattering basis for the Π symmetries is made up entirely of additional functions. The $(N+1)$ -particle closed-channel determinants are formed from a set of target pseudostates consisting of a $1\sigma_g$ orbital and a pseudoorbital together with an associated set of "scattering" functions. For the closed channels of Σ symmetry we used ten pseudostates, each of which has an associated set of seven scattering functions. In the Π symmetries we used six scattering functions with each of the eight pseudostates. Further, we have not included pseudoorbitals of Π symmetry in the closed-channel expansion for ${}^2\Sigma$ symmetries. Thus, configurations of the type $\pi_1^* \pi_2^* \sigma$, which may be important at lower energies, are not included.

As an initial step in this study we obtained ESE cross sections for comparison both with the results obtained with closed channels and as a preliminary test of our scattering and insertion basis sets. Our ESE integral cross sections are shown in Fig. 1 together with the ESE results of Collins, Robb, and Morrison.²⁸ The excellent agreement between these two sets of results indicates that our basis provides an accurate description of static-exchange scattering. Hence, any differences between our static-

exchange-polarization (SEP) cross sections and those of other studies should arise from the treatment of polarization.

In Figs. 2–4 we present our SEP integral cross sections for the ${}^2\Sigma_g$, ${}^2\Sigma_u$, and ${}^2\Pi_u$ symmetries, respectively. Also shown are the SEP results of Schneider and Collins¹⁵ in which an optical potential is used to include polarization effects and those of Gibson and Morrison⁶ whose treatment of polarization is based on a polarized orbital approach. For purposes of comparison we have included our ESE results. The ${}^2\Sigma_u$ and ${}^2\Pi_u$ cross sections of Figs. 3 and 4 show that the triplet-coupled target contributions to these cross sections are by no means negligible for this

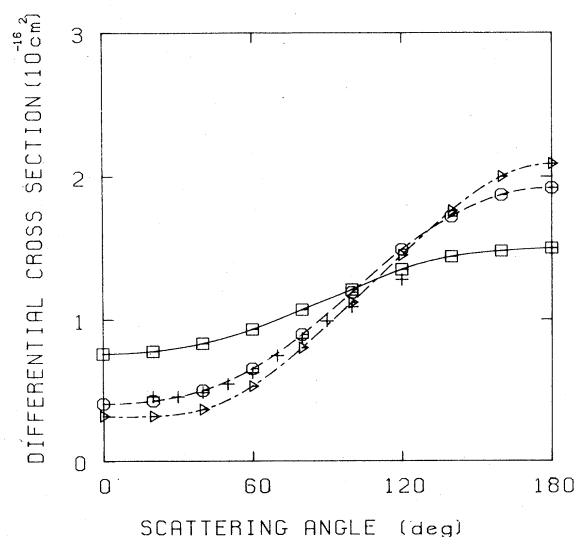


FIG. 6. Elastic differential cross sections (DCS) for $e\text{-H}_2$ scattering at 1 eV: present SE results (\square), present SEP results (\circ), SEP results from Ref. 6 (\triangle), measured values of Ref. 30 ($+$).

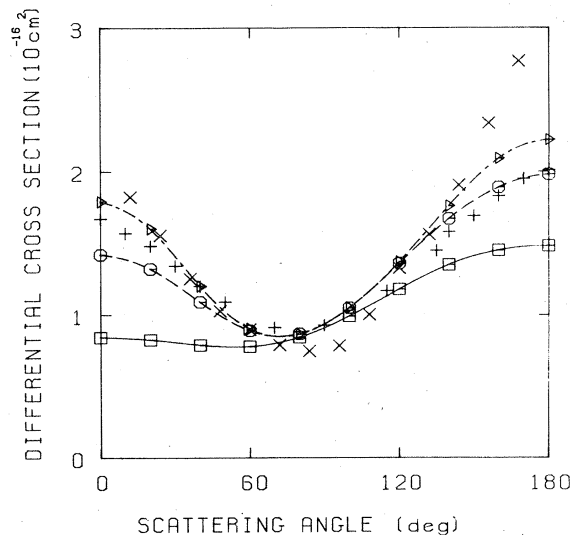


FIG. 7. DCS for $e\text{-H}_2$ scattering at 3 eV: present static-plus-exchange (SE) results (\square), present SEP results (\circ), SEP results from Ref. 6 (\triangle), measured values of Ref. 31 (+), measured values of Ref. 32 (\times).

energy range. For the Σ symmetries our SEP results are in quite reasonable agreement with those of the other two studies and a comparison shows that, with the exception of the lowest energy in the $^2\Sigma_g$ symmetry, almost all of the closed-channel effects are accurately taken into account. In Fig. 4 we see that our SEP results for the $^2\Pi_u$ symmetry are essentially identical to those of Schneider and Collins.⁵

Table II contains our total integral cross sections as well as those obtained by Gibson and Morrison⁶ and the measured values of Jones and Bonham.²⁹ The results of Schneider and Collins¹⁵ in Table II were interpolated onto an eV energy mesh using a cubic spline routine and include contributions from only the $^2\Sigma_g$, $^2\Sigma_u$, and $^2\Pi_u$ symmetries. The total cross sections are also shown in Fig. 5 along with our ESE results. Again, comparison shows that most of the closed-channel effects are properly accounted for by our method. Differential cross sections can provide greater insight into the scattering process and are a more stringent test of the theory than integral cross sections. We hence list our SEP differential cross sections in Table III. These results are shown in Figs. 6–8 for scattering energies of 1, 3, and 10 eV along with the corresponding ESE cross sections and the measured values of Linder and Schmidt,³⁰ Srivastava *et al.*,³¹ and Shyn and Sharp.³² Although Schneider and Collins¹⁵ did not report differential cross sections, we show results calculated from the T -matrix elements of Gibson and Morrison.⁶ For consistency, the results labeled Gibson and Morrison in Figs. 6–8 use the same partial-wave expansion as the present study, i.e., Σ and Π symmetries with $l \leq 3$. Although the differential cross sections so calculated are not highly converged in the extreme forward and backward directions at 10 eV, the associated integral cross section is converged to better than 1%. These figures show that the substantial differences in the cross sections due to the inclusion of polarization are reproduced by our method.

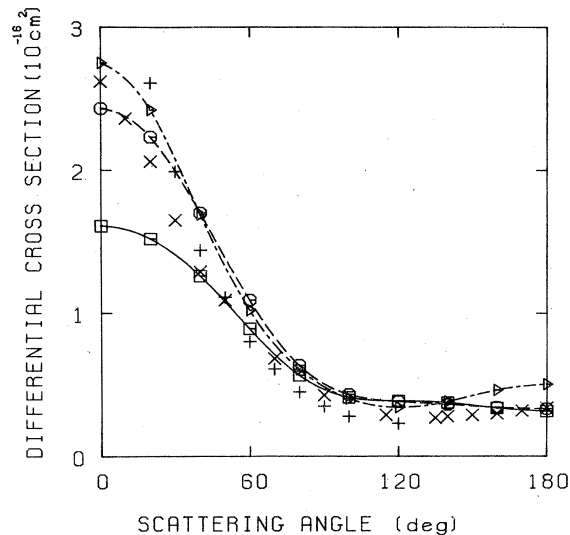


FIG. 8. DCS for $e\text{-H}_2$ scattering at 10 eV: present SE results (\square), present SEP results (\circ), SEP results from Ref. 6 (\triangle), measured values of Ref. 30 (+), measured values of Ref. 31 (\times).

Further, our SEP results are in very reasonable qualitative and quantitative agreement with measured values.

IV. CONCLUSIONS

In this paper we have reported a study designed to assess the effectiveness of our Schwinger multichannel formulation in representing polarization effects in low-energy electron-molecule collisions. We chose to obtain elastic integral and differential cross sections for $e\text{-H}_2$ collisions from 1 to 10 eV. It is worth noting that these calculations were implemented entirely in an L^2 basis. The integral cross sections show that our method can effectively and accurately represent most polarization effects without resorting to a large pseudostate expansion. Further, our differential cross sections were found to be in reasonably good agreement with existing measured values.

The SMC formulation has already been successfully applied to electronically inelastic $e\text{-H}_2$ scattering at the two-state static-exchange level of approximation. Extension of these studies to include the effects of closed channels on inelastic collisions is underway. Moreover, our method is designed to avoid the explicit construction of the closed-channel Green's function and to be applicable to closed-shell target molecules of arbitrary geometry. Further application of this approach to obtain elastic and electronically inelastic cross sections for a variety of molecular systems are underway.

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