

# Elastic cross sections and annihilation parameter for $e^+$ -H<sub>2</sub> scattering using the Schwinger multichannel method

Jorge L. S. Lino and José S. E. Germano

*Departamento de Física do Instituto Tecnológico de Aeronáutica—Centro Técnico de Aeronáutica,  
12228-900 São José dos Campos, SP, Brazil*

Euclimar P. da Silva

*Departamento de Física, Universidade Federal do Ceará, 60455-760 Fortaleza, Ceará, Brazil*

Marco A. P. Lima

*Instituto de Física, Unicamp, 13083-970 Campinas, São Paulo, Brazil*  
(Received 10 March 1998)

We report detailed results for positron-H<sub>2</sub> collisions obtained with the Schwinger multichannel method. Our calculations include annihilation parameter, differential, integral, and momentum transfer cross sections for energies below the positronium formation threshold. The calculations were carried out in the static-plus-polarization approximation with symmetry-resolved cross sections. Energy (temperature) dependence and symmetry-resolved contributions for the annihilation parameter  $Z_{\text{eff}}$  are also reported. Our *ab initio* integral cross sections are found to be in good agreement with the experimental data. [S1050-2947(98)04409-6]

PACS number(s): 36.10.Dr, 34.50.Gb

## I. INTRODUCTION

With the appearance of reliable magnetic traps, studies on low-energy matter-antimatter interactions have gained interest in the last few years. Particularly, substantial progress has been made in obtaining cross sections and annihilation rates for positron-molecule (atom) collision processes. Positron interactions with molecules can cause a variety of intriguing phenomena different from the electron case. The reason is that positrons can annihilate with an electron of the target during the process. The Coulombic attraction between positrons and electrons makes an enormous difference from the always repulsive interaction between electrons. As a result of such an attraction, positrons may form virtual positronium inside the molecule and if they have enough energy they can produce real positronium in the asymptotic region. Depending on the probability of finding a positron in the same position of an electron, the annihilation process can be weaker or stronger. The polarization potentials are always attractive and somehow always trying to put positrons and electrons together. Description of polarization interaction is very sensible because the static potential has opposite sign to the polarization potential. Therefore the positron-molecule problem is indeed more difficult to solve than the electron case, making the theoretical task of describing the phenomena very challenging. So, a suitable theory should be capable of dealing with several important aspects of the problem such as polarization effects, resonances, electronically inelastic scattering with several open and closed channels, positronium effects, and, if possible, applicable to nonlinear targets. A series of experiments involving positron impact with molecules has been done recently (see Refs. [1–3]) so that the theoretical calculations are extremely important for an adequate comparison. In particular, for the system analyzed here,  $e^+$ -H<sub>2</sub> scattering, some methods, such as the *R*-matrix (RM) method [4], the Kohn variational method (KVM) [5],

the distributed positron model (DPM) [6], and the Schwinger multichannel (SMC) method [7] have been used to calculate elastic integral cross sections. Accurate elastic differential cross sections (DCS) still remain an important and challenging endeavor. To test the potential of the SMC method we have calculated cross sections of molecules such as H<sub>2</sub> [7–9], CH<sub>4</sub> [7], and C<sub>2</sub>H<sub>4</sub> [10] by positron impact of low energy. In a recent paper, da Silva *et al.* [9] reported results for elastic integral cross sections and calculated the  $Z_{\text{eff}}$ , annihilation parameter of elastic positron-H<sub>2</sub>, using the SMC method at the static-plus-polarization level of approximation. In this present work we extend our previous calculations [9], to report on DCS, momentum transfer cross section (MTCS), integral cross section (ICS), and the annihilation parameter  $Z_{\text{eff}}$ . As we will see, our results are in very good agreement with available experimental data. In the present calculation we have used a more suitable procedure to choose the expansion basis functions to account for polarization effects. The SMC method does not incorporate real positronium formation, but it explicitly considers virtual positronium formation. In fact, full coupling of virtual positronium states is accounted for in the formalism. The precision depends only on how flexible the basis set is. Usually the molecular frame is the best frame to describe the collision process. Positroniums are better described in their center of mass. To remedy this problem, we have introduced several additional centers around the molecule. The choice of center positions and type of functions is a judicious choice and in some sense arbitrary. The strategy we are following involves the search of the lowest bound state of the composite (positron plus molecule) system. The remainder of this paper is organized into three sections. Section II gives a summary and some relevant theoretical details of the method. Section III describes details and results of our calculations on H<sub>2</sub>, and finally, Sec. IV presents our conclusions. Atomic units will be assumed throughout this paper, unless otherwise specified.

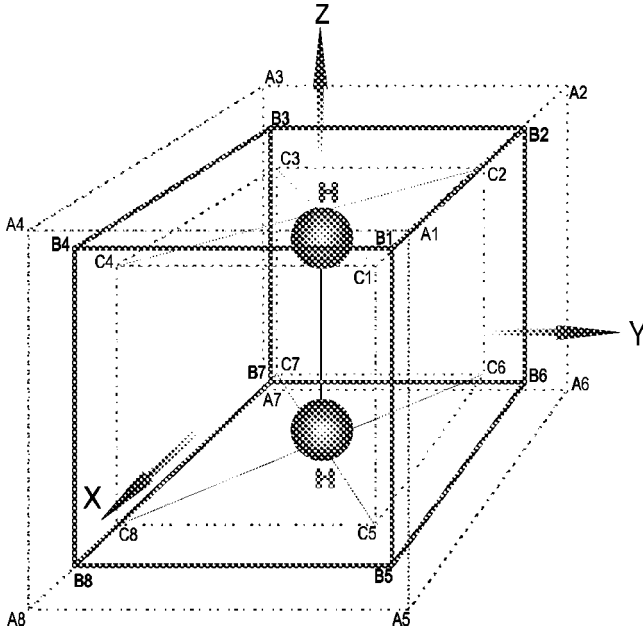


FIG. 1. Cubic distribution of extra basis function centers.

## II. SCHWINGER MULTICHANNEL METHOD

Details of the SMC method have been discussed elsewhere [7]. Here we will review a few important aspects of the method, which are essential to our present application. In the SMC method, the expression for the scattering amplitude is given by

$$[f(\vec{k}_f, \vec{k}_i)] = -\frac{1}{2\pi} \left( \sum_{mn} \langle S_{\vec{k}_f}^- | V | \chi_m \rangle (d^{-1})_{mn} \langle \chi_n | V | S_{\vec{k}_i}^- \rangle \right), \quad (1)$$

where

$$d_{mn} = \langle \chi_m | Q \hat{H} Q + PVP - VG_p^{(+)} V | \chi_n \rangle. \quad (2)$$

As in the original Schwinger principle for electrons [11], the trial scattering functions do not need to satisfy specific boundary conditions and hence they can be expanded in an  $L^2$  basis (square integrable basis). In these equations,  $S_{\vec{k}_i}^-$  is a product of a target state and a plane wave,  $V$  is the interac-

tion potential between a positron and the molecular target,  $\chi_n$  is an  $(N+1)$ -particle wave function used as variational trial function,  $\hat{H}$  is the total energy minus the full Hamiltonian of the system,  $N$  is the number of electrons in the target,  $P$  is a projector onto the energetically open electronic states of the target and  $Q$  onto the closed states, and  $G_p^{(+)}$  is the Green function projected on the  $P$  space. In our calculations, the static approximation can be obtained by defining  $P = |\phi_0\rangle\langle\phi_0|$ , where  $|\phi_0\rangle$  is the ground state of the target (for static approximation  $Q$  is made equal to zero). The polarization effects are included by defining  $Q = \sum_l |\phi_l\rangle\langle\phi_l|$ , where  $|\phi_l\rangle$  are excited states of the target, and the trial function set  $\chi_n$  is expanded from the static situation by including all simple products of  $|\phi_l\rangle$  and one-particle scattering functions (see Ref. [7]). The wave function obtained by the SMC method can be used to calculate the annihilation parameter  $Z_{\text{eff}}$ . Remembering that the annihilation parameter is related to the probability of an electron and a positron to be found in the same position we can write

$$Z_{\text{eff}}(\vec{k}_i) = \sum_{j=1}^N \langle \Psi_{\vec{k}_i}^{(+)}(\vec{r}_1, \dots, \vec{r}_N, \vec{r}_p) | \delta(\vec{r}_j - \vec{r}_p) | \Psi_{\vec{k}_i}^{(+)}(\vec{r}_1, \dots, \vec{r}_N, \vec{r}_p) \rangle. \quad (3)$$

This quantity can be evaluated with the help of the SMC  $(N+1)$ -particle scattering wave function which is given by [9]

$$|\Psi_{\vec{k}_i}^{(+)}\rangle = \sum_{m,m'} |\chi_{m'}\rangle (d^{-1})_{mm'} \langle \chi_m | V | S_{\vec{k}_i}^- \rangle. \quad (4)$$

As in Ref. [9], the reported annihilation parameters are obtained through an angular average of Eq. (3).

## III. PROCEDURE AND RESULTS

For impact energies below real positronium formation, the SMC method carries the important aspects of the collision process, including the possibility of virtual positronium formation. As mentioned before, positroniums are better described in their center of mass and not in the molecular center. To remedy this problem we have introduced several

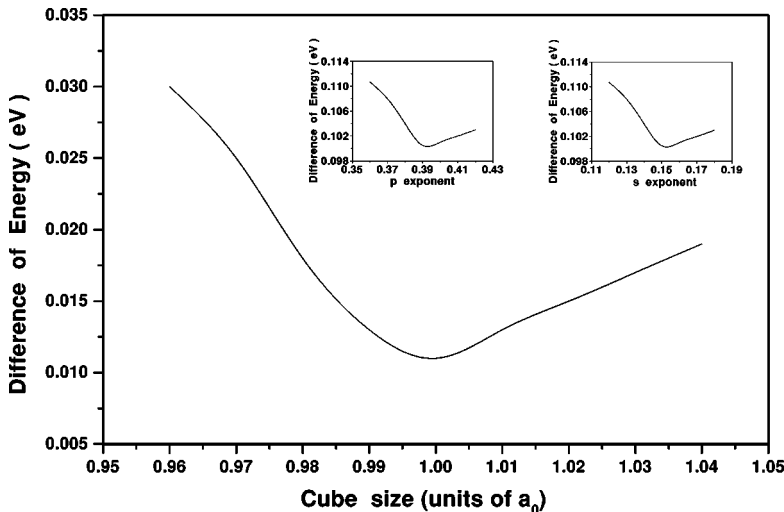
FIG. 2. Optimization of the cube size and choices of  $s$  and  $p$  functions.

TABLE I. Differential cross sections for positron-H<sub>2</sub> collisions (in units of  $a_0^2$ ).

Angle (deg)	0.136 eV	1.36 eV	2.72 eV	3.5 eV	4.08 eV	4.5 eV	6.9 eV
0	4.001	1.705	1.848	1.738	1.621	1.454	1.311
10	3.981	1.664	1.771	1.654	1.536	1.223	1.216
20	3.922	1.547	1.554	1.423	1.304	0.904	0.965
30	3.892	1.369	1.240	1.096	0.981	0.575	0.643
40	3.707	1.150	0.890	0.744	0.641	0.299	0.344
50	3.563	0.918	0.564	0.431	0.349	0.115	0.135
60	3.404	0.698	0.308	0.203	0.147	0.026	0.033
70	3.238	0.510	0.140	0.071	0.041	0.010	0.019
80	3.072	0.363	0.055	0.022	0.012	0.035	0.056
90	2.909	0.257	0.027	0.024	0.029	0.072	0.107
100	2.756	0.185	0.027	0.046	0.061	0.104	0.151
110	2.614	0.138	0.037	0.069	0.091	0.124	0.178
120	2.486	0.107	0.04	0.084	0.109	0.134	0.191
130	2.375	0.087	0.05	0.090	0.117	0.137	0.197
140	2.282	0.072	0.05	0.092	0.119	0.138	0.202
150	2.208	0.061	0.05	0.092	0.118	0.138	0.207
160	2.154	0.054	0.06	0.092	0.117	0.137	0.214
170	2.122	0.049	0.06	0.094	0.117	0.137	0.219
180	2.111	0.048	0.06	0.096	0.117	0.137	0.221
ICS	37.173	5.773	3.564	3.130	2.974	2.770	2.632
MTCS	33.275	2.820	1.232	1.276	1.458	1.472	2.062

additional centers around the molecule. With this in mind, we have established (arbitrarily) a cubic distribution of centers with the molecule inside it (see Fig. 1). In principle the adopted geometrical figure could be anything. We used a cubic distribution because it is more convenient for the SMC computer code in terms of symmetry exploration. The functions used for each center are chosen by searching the lowest bound state of the composite (positron plus molecule) system. The idea can be better understood with the help of Fig. 1. First, we considered the molecule inside of a cubic distribution of basis function centers situated at  $B_1, \dots, B_8$  positions. We then place Cartesian Gaussian functions of types

“ $s$ ” and “ $p$ ” on each corner ( $B_1, \dots, B_8$ ) of the cube. With the cube in the initial position, we optimized the values of the  $s$  and  $p$  exponents, through the minimization of the energy of the composite positron plus molecule system (by simple diagonalization of the Hamiltonian matrix of the composite). The optimized values for the Gaussian exponents were then used to find a new “best size” of the cube. This procedure is repeated until convergence is achieved. With this approach, we have found the corner of the cube as  $X = 1.0a_0$ ,  $Y = 1.0a_0$ ,  $Z = 1.0a_0$  and the exponents of functions  $s$  and  $p$  as 0.15 and 0.39, respectively (see Fig. 2). The three curves, in Fig. 2, were obtained by varying each parameter (size of the cube or  $s$  or  $p$  exponents) with the other two parameters fixed in their best values. We have observed that the optimization of these extra center positions and of the Cartesian Gaussian exponents represent an important and necessary step in obtaining converged cross sections for positron scattering [16]. Our calculations for H<sub>2</sub> were made considering the  $D_{2h}$  point group and we included contributions to the cross sections and to the annihilation parameters from all eight symmetries,  $A_g$ ,  $A_u$ ,  $B_{1u}$ ,  $B_{2u}$ ,  $B_{3u}$ ,  $B_{1g}$ ,  $B_{2g}$ , and  $B_{3g}$  of this group. In this work, the target wave function was obtained by a Hartree-Fock calculation using the same basis set of Ref. [9]. For the description of scattering wave function and of polarization effects we included the above-mentioned  $s$  and  $p$  functions in the cube and one  $d$  function with exponent 0.005 at the center of mass of the molecule. In our basis, the induced polarizability was determined to be

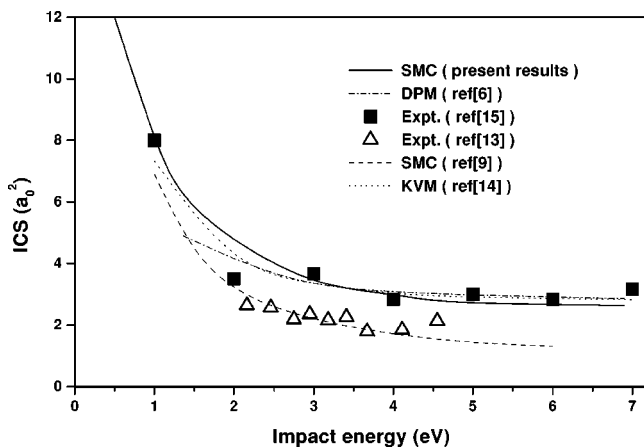


FIG. 3. Elastic integral cross sections (ICS) for  $e^+$ -H<sub>2</sub>. Present results: solid line; results of the SMC method of Ref. [9]: dashed line; results of DPM method of Ref. [6]: dot-dashed line; results of the Kohn variational method (KVM) of Ref. [14]: dotted line; experimental data of Ref. [15]: full squares; experimental data of Ref. [13]: triangles.

TABLE II. Values of  $Z_{\text{eff}}$  at room temperature.

Expt. (Ref. [13])	SMC (Ref. [9])	Our result
14.7	13.63	14.82

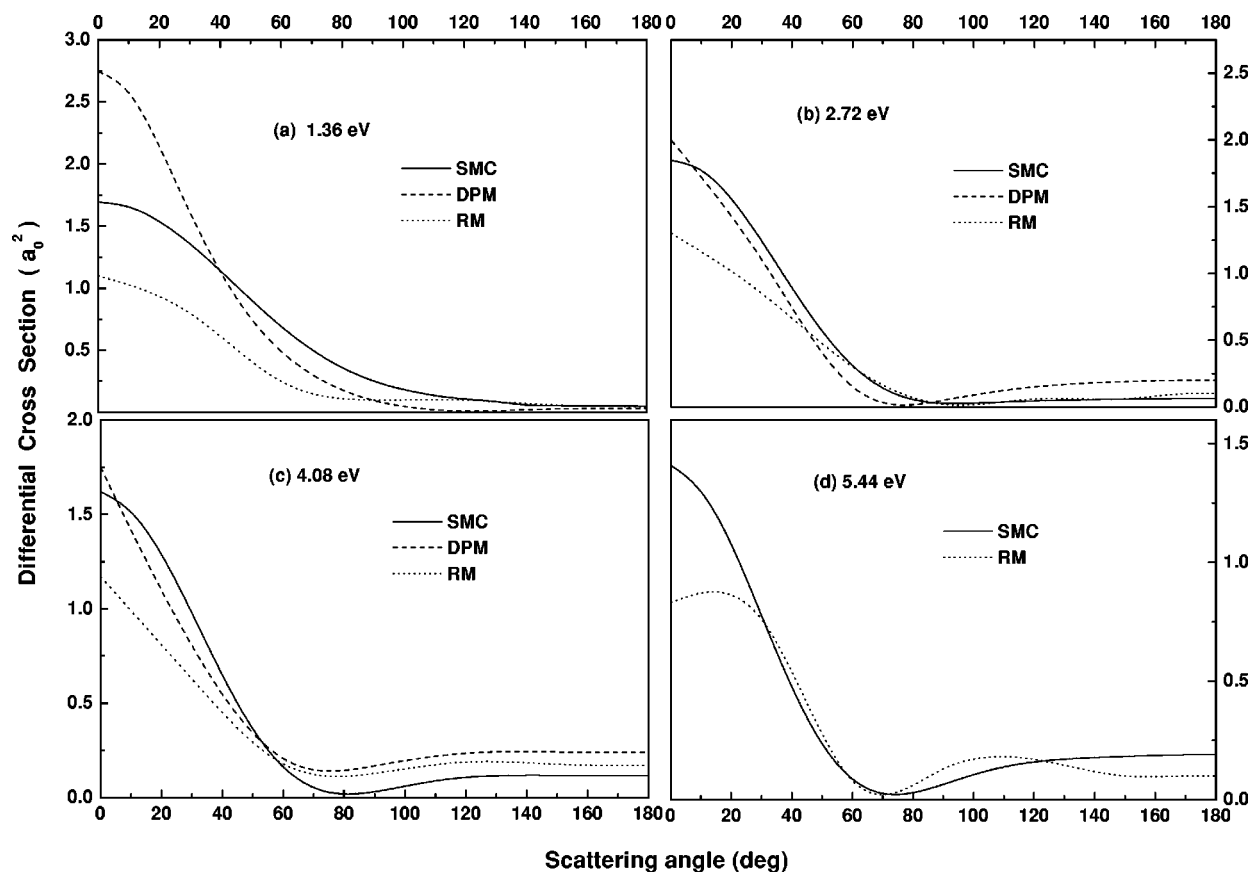


FIG. 4. Elastic differential cross sections (DCS) for the  $e^+ - \text{H}_2$  at 1.36, 2.72, 4.08, and 5.44 eV. Present results (SMC): solid line; results of DPM method of Ref. [6]: dashed line; results of the  $R$ -matrix method of Ref. [4]: dotted line.

$5.221a_0^3$ . Again, this result compares favorably well with the theoretical result  $5.173a_0^3$  of Ref. [6] and the experimental result  $5.179a_0^3$  of Ref. [12]. In the present calculation we used 78 Cartesian Gaussian functions and a total number of 7312 configurations (in our earlier paper [9] we used 64 functions and a total of 4096 configurations) to expand the scattering wave function. In order to check the numerical integrations in the momentum space of the present SMC application, we tested the results with several quadratures until full convergence was achieved. The DCS for several energies are listed in Table I with the total integrated cross sections obtained when contributions from all eight symmetries are included. In Fig. 3 we show our ICS obtained with the SMC method in comparison with experimental and other theoretical results. Our ICS agree better with the experimental data of Hoffman *et al.* [15]. Figure 3 shows that the present results (obtained with the same SMC) are considerably different from those obtained in our earlier calculations [9], but they are in better agreement with other theoretical results. We believe this is an indication that our choice for basis functions is now more adequate. Furthermore, as a consequence, our annihilation parameter  $Z_{\text{eff}}$  is now also very good in comparison with experimental datum at room temperature (see Table II). Since we are interested also in computing DCS for  $e^+ - \text{H}_2$  at low impact energies, a comparison of SMC with other theoretical results would be useful. In Figs. 4(a), 4(b), 4(c), and 4(d), we present our results of DCS for energies 1.36, 2.72, 4.08, and 5.44 eV, respectively. For

these energies we compared the SMC results with the DPM [6] and the RM [4] methods. With this good agreement between our ICS and DCS with other theoretical results, we have an encouraging indication that the physics assumptions involved in our procedures are substantially correct.

Finally in Fig. 5, we present the energy dependence of symmetry-resolved annihilation parameter. The symmetries  $B_{2u}$  and  $B_{3u}$ , and  $B_{2g}$  and  $B_{3g}$  are degenerate and only one of them is shown in the figure. As we have found in

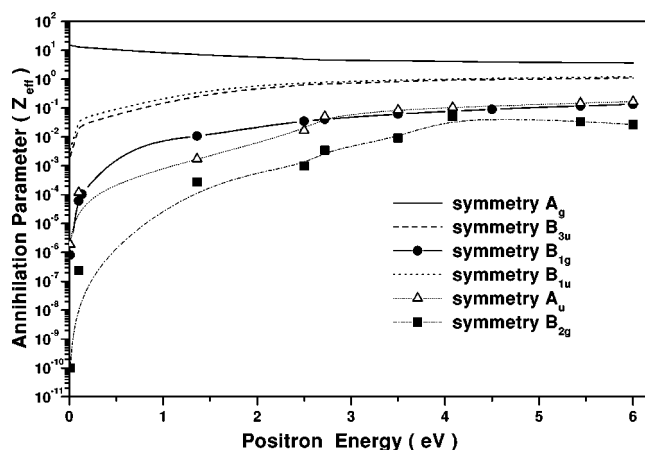


FIG. 5. Energy dependence of symmetry-resolved annihilation parameter  $Z_{\text{eff}}$ .

$e^+$ -C<sub>2</sub>H<sub>4</sub> scattering [10] the main contribution for the  $Z_{\text{eff}}$  comes from the  $A_g$  symmetry.

#### IV. CONCLUSIONS

In this paper we have reported an application of the Schwinger multichannel method to low-energy positron collisions with the target H<sub>2</sub>. Using this system we have developed a procedure of making a judicious choice of the expansion basis set for the description of polarization effects. Differential cross sections at the static-plus-polarization level of approximation have been reported for energies below positronium formation. Our results were found to be in good agreement with other theoretical results and with the experi-

mental data of Hoffman *et al.* [15]. The existing discrepancy between experimental data sets needs further investigation. The present study helps to demonstrate the utility of this approach and represents considerable progress toward obtaining *ab initio* differential cross sections and the  $Z_{\text{eff}}$  parameter for a variety of other molecular targets.

#### ACKNOWLEDGMENTS

One of us (J.L.S.L.) acknowledges financial support from the Fundação de Amparo à Pesquisa do Estado de São Paulo (Fapesp), São Paulo, Brazil. J.S.E.G. and M.A.P.L. acknowledge financial support from Conselho Nacional de Pesquisa e Desenvolvimento (CNPq).

- 
- [1] See, for example, T. S. Stein, M. Harte, J. Jiang, W. E. Kauppila, C. K. Kwan, H. Li, D. A. Przybyla, and S. Zhou (unpublished); see also D. A. Przybyla *et al.*, Phys. Rev. A **55**, 4244 (1997).
- [2] T. J. Murphy and C. M. Surko, Phys. Rev. Lett. **67**, 2954 (1991); see also G. Laricchia, in *The Physics of Electronic and Atomic Collisions*, edited by L. J. Dube, B. A. Mitchell, W. McConkey, and E. Brion, AIP Conf. Proc. No. 360 (AIP, New York, 1995), p. 385.
- [3] D. J. Day, G. Laricchia, and M. Charlton, Hyperfine Interact. **73**, 2017 (1992).
- [4] G. Danby and J. Tennyson, J. Phys. B **23**, 1005 (1990); **23**, 2471 (1990).
- [5] C. E. McCurdy, T. N. Rescigno, and B. I. Schneider, Phys. Rev. A **36**, 2061 (1987).
- [6] T. L. Gibson, J. Phys. B **25**, 1321 (1992).
- [7] J. S. E. Germano and M. A. P. Lima, Phys. Rev. A **47**, 3976 (1993).
- [8] J. L. S. Lino, J. S. E. Germano, and M. A. P. Lima, J. Phys. B **27**, 1881 (1994).
- [9] E. P. da Silva, J. S. E. Germano, and M. A. P. Lima, Phys. Rev. A **49**, R1527 (1994).
- [10] E. P. da Silva, J. S. E. Germano, and M. A. P. Lima, Phys. Rev. Lett. **77**, 1028 (1996).
- [11] K. Takatsuka and V. McKoy, Phys. Rev. A **24**, 2473 (1981).
- [12] W. Kolos and L. Wolniewicz, J. Chem. Phys. **43**, 2429 (1965).
- [13] M. Charlton, T. C. Griffith, G. R. Heyland, and G. L. Wright, J. Phys. B **16**, 323 (1983).
- [14] E. A. G. Armour and M. Plummer, J. Phys. B **23**, 3057 (1990).
- [15] K. R. Hoffman, M. S. Dababneh, Y. F. Hsieh, W. E. Kauppila, V. Pol, J. H. Smart, and S. Stein, Phys. Rev. A **25**, 1393 (1982).
- [16] E. P. da Silva, J. S. E. Germano, J. L. S. Lino, C. R. C. Carvalho, A. P. P. Natalense, and M. A. P. Lima, Nucl. Instrum. Methods Res. B **143**, 140 (1998).