PHYSICAL REVIEW A **72**, 042709 (2005)

Correlated dipole-polarized basis in Schwinger's principle for elastic positron-hydrogen collisions

Arijit Ghoshal[1] and Puspajit Mandal[2]
[1]*Department of Mathematics, Suri Vidyasagar College, Suri 731 101 West Bengal, India*
[2]*Department of Mathematics, Visva-Bharati University, Santiniketan 731 235 West Bengal, India*

(Received 13 January 2005; revised manuscript received 22 April 2005; published 14 October 2005)

Definitive results for elastic positron-hydrogen collisions are obtained using the Schwinger variational principle in the momentum space at low and intermediate energies corresponding to momenta in the range $k_i=0$–3.5 atomic units. The discrete basis set used in the calculation makes allowance for long-range dipole polarization, atomic distortion, and infinite-order short-range positron-electron correlation. Results for the scattering parameters, such as the scattering length, phase shifts for all significant partial waves, and total cross section, are in conformity with other accurate variational and nonvariational calculations available in the literature.

DOI: 10.1103/PhysRevA.72.042709 PACS number(s): 34.80.Gs, 34.70.+e, 36.10.Dr

I. INTRODUCTION

Since the early developments of quantum mechanics, variational methods have proved to be very useful techniques for solving bound-state problems. It was only much later that the application of variational principles in quantum collision phenomena was proposed by Hulthen [1], Tamm [2], Schwinger [3], and Kohn [4]. A number of methods followed their work [5].

Variational principles applicable to quantum collision theory can conveniently be classified into two categories, namely, differential and integral forms. The first are based directly on the solution of differential equations resulting from the corresponding Schrödinger equation and require the trial functions to satisfy the boundary conditions of the problems concerned. The Kohn-Hulthen variational principle [1,4] is based on the differential aspect of the variational principles. The integral forms, on the other hand, are derived from the corresponding Euler-Lagrange (or Lippmann-Schwinger) integral equations and therefore the boundary conditions, being taken into account through the Green's function, need not be incorporated into the trial functions. In the following sections we shall discuss our primary interest of study, the Schwinger variational principle [3], relying on the corresponding integral equations.

About 57 years ago Schwinger [3] proposed a variational technique for solving Schrödinger's equation in its integral form. The method was analyzed in different ways by Blatt and Jackson [6], Kato [7], and Blatt and Biedenharn [8] for single- and multichannel scattering problems. Excellent reviews of the method are given in the monographs of Mott and Massey [9], Moiseiwitsch [10], Joachain [11], Burke [12], Bransden [13], Schmid and Ziegelmann [14], Nesbet [15], and Newton [16].

The first application of Schwinger's variational method to atomic collisions was made by Altshuler [17]. He used a set of polynomial functions to investigate the scattering of electrons by square-well and Yukawa potentials as well as the static potential of the hydrogen atom. He further made a comparative analysis of the results for the scattering phase shifts, amplitudes, and total cross sections determined by the Schwinger variational method, Kohn's method [9,10,15], and the second Born approximation, and arrived at the following points. (i) Schwinger's variational phases are closer to the exact ones than Kohn's phases, when the same trial functions are used in both cases. (ii) Scattering amplitudes obtained by Schwinger's method are better than those from the second Born approximation. Schwartz [18] also carried out a comparative analysis of the Schwinger phase shifts of S-wave electron scattering by Yukawa potentials $V(r)=-2e^{-r/r_0}$ with the corresponding Kohn variational results and made the following conclusions: (a) The Schwinger variational method leads to smooth curves which converge as the number of terms in the trial function increases; (b) The Kohn phases converge much faster and their values at the same number of terms in the trial function are more accurate.

As a matter of fact, the point (b), which does not agree with the earlier conclusions of Altshuler [17], has led to differing opinions about the quality of the phase shifts produced by the Schwinger variational method and Kohn's method (Abdel-Raouf [19]).

Saraph [20] showed with a trial expansion space of three components that the singlet and triplet scattering lengths of electron hydrogen scattering agree well with those calculated by John [21] using exact numerical integration.

During the last three decades, McKoy and co-workers, in a number of applications in the field of atomic and molecular collisions [22–43], have demonstrated the efficiency of the Schwinger variational principle and emphasized that the Schwinger variational principle provides better results when a discretization technique is employed. Indeed, Takatsuka and McKoy [27] compared their Schwinger results with those determined by Harris and Michels [30] and Nesbet and Oberoi [31] using anomaly-free variational methods, and established faster convergence of Schwinger's phase shifts compared with other variational methods.

Important investigations using the Schwinger variational principle were carried out by many authors within the framework of the separable approximation. Mention may be made of the findings of Sugar and Blankenbecler [44], Sloan and Adhikari [32], Zubarev and co-workers [33,34], Hahn [40], Nuttal [35], Watson [42], Moiseiwitsch [10,45], and Maleki and Macek [38].

1050-2947/2005/72(4)/042709(13)/$23.00

It is also interesting to discuss the application of the Schwinger variational principle to bound-state problems, which was originally explored in the work of Sugar and Blankenbecler [44] and strongly emphasized by Schwartz and Zemach [36] through their successful treatment of Bethe-Salpeter problems. Singh and Stauffer [46] and Zubarev [47] presented the explicit formulation of this method for the Bethe-Salpeter problems. Because of the difficulties associated with the evaluation of matrix elements involving the Green's function operators, the Schwinger variational principle has seldom been applied to atomic, molecular, and nuclear bound-state problems, where the superiority of the Rayleigh-Ritz method is beyond any doubt. However, Maleki and Macek [37,38] indicated the usefulness of the Schwinger variational principle within the framework of quantum defect theory for the calculation of bound and continuum states of high Rydberg atoms.

A number of important contributions toward various aspects and applications of the Schwinger variational principle have been made during the last 30 years. In particular Hahn [40] generalized the Schwinger principle by projecting the Lippmann-Schwinger equation with an arbitrary operator W. Different choices of W are then considered; some of the results obtained by Takatsuka and McKoy [26,28] are shown to follow special choices of W. In important work, Moiseiwitsch [45] proved that the linear algebraic equation method (Sneider and Collins [48]) for evaluating a phase shift from the integral equation for scattering is equivalent to using the Schwinger variational principle. He further showed that a modification of the linear algebraic method ensures a variational bound in the phase shifts for potentials having a definite sign at all points.

In a further development, Domcke [41] showed that the Schwinger variational principle is a variational approximation for the poles of the analytically continued T matrix (or S matrix) and applied it to calculate the bound states, virtual states, and resonances of a simple model problem, namely, the S-wave scattering by an attractive square-well potential, to obtain accurate results with few basis functions. In similar studies, Watson [42] quite independently obtained accurate resonance energies and total and partial widths for multichannel scattering problems by considering the complex momentum phase for the poles of the Schwinger T matrix.

However, of late certain anomalies of Schwinger variational phase shifts in momentum space were studied by Adhikari [39]. Adhikari demonstrated that these anomalies were related to the appearance of continuum bound states in approximate calculations and had no relevance in a realistic calculation. He observed that the anomalies were in no way related to the spurious singularities that had appeared in the Kohn variational calculation.

Finally, a major development toward the applications of the Schwinger variational principle to positron-hydrogen collisions was made by Roy and Mandal [49] and Kar and Mandal [50,51]. Roy and Mandal [49] utilized a type of correlated function in the form

$$\xi_m(r_1,r_{12}) = \exp(-\alpha_m r_1 - \chi\, r_{12})/(a + b\, r_{12})^{m_0}, \qquad m = 1,2,\ldots,N, \quad m_0 = 1,2,\ldots, \tag{1}$$

within the framework of the Schwinger variational principle to study elastic positron-hydrogen collisions, in which $\vec{r}_1$ denotes the position vector of the positron, $\vec{r}_2$ that of the electron, and $\vec{r}_{12}=\vec{r}_1-\vec{r}_2$, relative to the infinitely heavy proton at the center of the coordinate system. They were able to report accurate results for elastic scattering for all partial waves below 10.2 eV using only $n=4$ terms.

Subsequently Kar and Mandal [50] employed a correlated basis set

$$u_m(\vec{r}_1,\vec{r}_2) = (-1)^{m-1}\Phi_i(\vec{r}_1,\vec{r}_2)\xi_m(r_1,r_{12}), \tag{2}$$

where the plane-wave states in the incident channel are

$$\Phi_i(\vec{r}_1,\vec{r}_2) = \exp(i\vec{k}_i\cdot\vec{r}_1)\,\phi_i(\vec{r}_2), \tag{3}$$

and the correlation function $\xi_m(r_1,r_{12})$ is given by

$$\xi_m(r_1,r_{12}) = \exp(-\alpha_m r_1 - \chi\, r_{12})/(a + b\, r_{12})^{m_0-1/2}, \qquad m = 1,2,\ldots,N, \quad m_0 = 1,2,\ldots. \tag{4}$$

They reported accurate results for the elastic scattering for all partial waves below 30 eV using only $N=8$ terms in the basis. The basis functions were, however, of no use for higher energies.

These findings are in conformity with the definitive Kohn-Hulthen variational results and other calculations available in the literature (Schwartz [52], Bhatia *et al.* [53,54], Chan and Fraser [55], Chan and McEachran [56], Humberston [57], Brown and Humberston [58], Mitroy [59], Winick and Reinhardt [60]).

A noteworthy deficiency in the above choice of correlated basis sets (1) and (3) is that none of them explicitly includes the effect of atomic distortion, which has been found to play a vital role in determining accurate results, although both of the basis sets duly take care of electron-positron correlation.

The main objective of our present investigation is to propose a discrete basis set that will be applicable to low as well as intermediate energies for elastic positron-hydrogen collisions. The present Schwinger variational calculation is an extension of the earlier theoretical methodology incorporating a trial function that includes a dipole polarization-response term. In this work, we use an exponential basis, while all of our earlier publications dealt with inverse correlated basis functions. For elastic positron-hydrogen scattering, the present calculation seems to work better at all incident energies. Our investigation endeavors to make an in-depth study of this process and performs reliable predictions of the scattering parameters such as the scattering length, phase shifts for all significant partial waves, and total cross sections.

The plan of the paper is as follows. In Sec. II we discuss the underlying theory of choosing the basis set. Section III is devoted to the discussion of the results as obtained by the present calculation. Finally in Sec. IV we make our concluding remarks.

II. THEORY

We know that short-range correlations play an important role in determining the detailed nature of atomic, molecular, and nuclear collisions. Proper account of electron-electron correlation in bound-state calculations of atoms and molecules is of vital importance for obtaining definitive answers to the structural properties. For positron-atom and positron-molecule collisions, in addition to the short-range positron-electron correlation, there occur distortion of the target atom and the long-range positron-induced polarization of the target charge cloud, which are of much greater significance in predicting accurate scattering parameters. Since these two interactions are attractive and act in opposition to the repulsive static interaction, any noteworthy calculation must take proper account of these interactions to obtain meaningful results.

In this work, we investigate the elastic positron-hydrogen collisions and study the usefulness of incorporating the effects of dipole distortion of the atom by means of a polarization response function in addition to the exponential correlation in the basis of Schwinger variational principle. Such prescriptions have a parallel in polarization pseudostates introduced by Damburg and Karule [61] in electron-atom scattering and intensively used in electron-molecule scattering by others.

We choose an exponential correlated basis set as

$$u_m(\vec{r}_1,\vec{r}_2) = \Phi_i(\vec{r}_1,\vec{r}_2)\xi(\vec{r}_1,\vec{r}_2) \tag{5}$$

in which the correlation function is taken in the form

$$\xi(\vec{r}_1,\vec{r}_2) = (1 - e^{-pr_1})e^{-\beta r_2-\gamma r_{12}}r_1^{m_0-1} + G_d(\vec{r}_1,\vec{r}_2),$$

$$G_d(\vec{r}_1,\vec{r}_2) = \Theta(r_1 - r_2)r_2^{-1}f_d(r_1,r_2)\cos\alpha, \quad m_0 = 1,2,3,4, \tag{6}$$

where p, β, and γ are the nonlinear variational parameters to be optimized with $\cos\alpha=\hat{r}_1\cdot\hat{r}_2$ and $\Theta(y)=1$ for $y>0$, $\Theta=0$ otherwise. The function f_d is found to satisfy [62]

$$\left(\frac{d^2}{dr_2^2} - \frac{2}{r_2^2} + \frac{2}{r_2} - 1\right)f_d(r_1,r_2) = \left(\frac{4}{\pi}\right)^{1/2}\frac{r_2^2}{r_1^2}e^{-r_2} \tag{7}$$

with the solution

$$f_d(r_1,r_2) = -\left(\frac{1}{\pi}\right)^{1/2}\frac{r_2^2}{r_1^2}\left(1 + \frac{r_2}{2}\right)e^{-r_2}. \tag{8}$$

It is to be mentioned that the potential generated by the function

$$G_d(\vec{r}_1,\vec{r}_2) = \Theta(r_1 - r_2)r_2^{-1}f_d(r_1,r_2)\cos\alpha$$

is of the form

$$\begin{aligned} U_d(r_1) &= -\frac{1}{r_1^4}\Bigg[\frac{9}{2} - \frac{2}{3}e^{-2r_1} \\ &\quad\times\left(r_1^5 + \frac{9}{2}r_1^4 + 9r_1^3 + \frac{27}{2}r_1^2 + \frac{27}{2}r_1 + \frac{27}{4}\right)\Bigg] \\ &\to \begin{cases} 0 & \text{as } r_1 \to 0, \\ -\dfrac{9}{2r_1^4} & \text{as } r_1 \to \infty. \end{cases} \end{aligned} \tag{9}$$

The noteworthy feature of our basis set is that it accounts well for dipole distortion effects, including particularly long-range polarization by means of the dipole distortion term $G_p(\vec{r}_1,\vec{r}_2)$ in addition to the infinite-order positron-electron correlation being taken into account by the term $e^{-\gamma r_{12}}$. Temkin and Lamkin [63] first used this dipole distortion term in the trial function of Kohn's variational method to study electron-hydrogen collisions and reported reasonably accurate results. Furthermore, existence of the term $e^{-\beta r_2}$ in our basis has made it possible to have holdover effects due to distortion of the atom by the incoming positron.

We have used the above basis set in the Schwinger variational amplitude as obtained by Roy and Mandal [49], and Kar and Mandal in the momentum space [50]:

$$[A_{fi}^{(L)}(k_f,k_i)] = \sum_{m,n}\sum_{p,q} A_{fm}^{(L)}(k_f,k_i)D_{mn}^{(L)(pq)^{-1}}A_{ni}^{(L)}(k_f,k_i) \tag{10}$$

which is a function of the scattering energies for any partial wave L. Here $A_{fm}^{(L)}(k_f,k_i)$,$A_{ni}^{(L)}(k_f,k_i)$ are the input two-body amplitudes and $D_{mn}^{(L)(pq)^{-1}}$ are the inverse matrix elements of the double-scattering matrix $D_{mn}^{(L)(pq)}$. The evaluation of the relevant amplitudes is shown in the Appendix. These are obtained in closed analytic forms.

III. RESULTS AND DISCUSSIONS

We have evaluated the stationary scattering amplitude (10) using correlated basis functions (5) and have optimized the nonlinear variational parameters p, β, and γ, by setting $m_0=1$. Our well-defined prescription of optimization has been to find the stationary values of the scattering amplitude (10) for a reasonable range of values of the nonlinear variational parameter p given the other two nonlinear variational parameters β and γ. Using the basis set (5), the "input" two-body amplitudes are conveniently obtained as a function of the incident energy for each partial wave l. The effects of the dominant interactions for low-energy collisions are taken care of by the correlated basis functions which are quite flexible.

A. Zero-energy scattering; scattering length

The scattering length plays a fundamental role in zero-energy scattering. At low energies the scattering occurs predominantly in the S wave, and the scattering length gives a measure of scattering. This quantity has been calculated very accurately by using variational methods [53,64,65] and provides a severe test for the validity of our calculation in the zero-energy region. It provides also a direct check on the

TABLE I. Stationary values of the *S*-wave phase shifts, the ratio $(\tan\,\delta_0)/k_i$ along with the nonlinear variational parameters p, β, and γ as functions of the incident positron energy k_i.

k_i (a.u.)	p	β	γ	δ_0	$\tan\,\delta_0/k_i$
0.09	1.5	0.4436	0.0303	0.1396	1.5516
0.08	1.4	0.4586	0.0267	0.1290	1.6124
0.07	1.4	0.4724	0.0232	0.1171	1.6735
0.06	1.4	0.4892	0.0197	0.1041	1.7348
0.05	1.4	0.5043	0.0164	0.0899	1.7977
0.04	1.4	0.5151	0.0131	0.0742	1.8564
0.03	1.4	0.5198	0.0100	0.0575	1.9166
0.02	1.4	0.5335	0.0068	0.0395	1.9768
0.01	1.3	0.5500	0.0035	0.0203	2.0328
0.007	1.3	0.5626	0.0025	0.0144	2.0547
0.005	1.3	0.5742	0.0018	0.0103	2.0673
0.003	1.3	0.5841	0.0011	0.0062	2.0818
0.001	1.3	0.5894	0.0004	0.0021	2.0977
0.000					(−2.10)[a]

[a] Scattering length $a_s = -\lim_{k_i\to 0}[(\tan\,\delta_0)/k_i]$, $\delta_0 = S$-wave phase shift.

reliability of the basis set due to the fact that in our approach the scattering information is supposed to be included in the basis set.

Table I lists the ratio $K_0 = (\tan\,\delta_0)/k_i$ as obtained by the present calculation as a function of the incident positron energy. The limit of this term as $k_i \to 0$ gives the value of the scattering length. Figure 1 shows the graphical representation of the convergence of this ratio K_0 with decreasing energy. The convergence is linear and monotonic. We have, however, used a parabolic extrapolation formula to find the limit of $(\tan\,\delta_0)/k_i$ as $k_i \to 0$ and obtained the accurate value of the scattering length. It is important to note that the effect of distortion of the target atom by the incoming positron for *S*-wave e^+-H scattering dominates over the positron-electron correlation at the zero-energy level. This effect of distortion is maximum near zero energy while the effect of correlation is negligible therein as is evident from a comparison of the variational distortion parameter β and correlation parameter γ in Table I.

B. Positron energy below 13.6 eV

The problem of elastic scattering in this energy region is generally viewed in three different aspects based upon opening and nonopening of scattering channels as follows: (i) Scattering below the positronium formation threshold 6.8 eV—only the elastic scattering is energetically possible in this region; (ii) Scattering in the Ore gap (6.8–10.2 eV)—both elastic and positronium formation channels are open in this energy region; (iii) Scattering above the first excitation threshold but below the ionization threshold (10.2–13.6 eV)—besides elastic scattering and positronium formation, all excitation channels are open.

The problems of elastic scattering for the cases (i) and (ii) are considered to be solved with accurate values of the phase shift and the differential cross section now available in the literature. In the elastic region (i), we have the accurate variational results of Schwartz [52], Kleinman *et al.* [66], Armstead [67], Bhatia *et al.* [53,54], and Roy and Mandal [49]. These results stand as benchmark and provide the standard by which the accuracy of other methods of approximation is judged. In the Ore gap region (ii), studies of elastic scattering were elaborately made by Humberston and coworkers [57,58], Gien [68,69], Mitroy [59], Chan and Fraser [55], Kar and Mandal [50]. However these authors except those of [50] limited their calculations to only a few lower partial waves. As a consequence, the elastic differential cross section (the evaluation of which requires higher partial-wave contributions) has been studied in detail only by the authors of Refs. [49,50]. Above the positronium formation threshold [case (iii)], the reported works are not as numerous as in the previous two cases. It is basically due to the fact that an infinite number of channels are open in this energy region, and it becomes a difficult task to take into account the effects of all such channels in order to obtain accurate results. Recently Kar and Mandal [50] have reported Schwinger variational results in this energy region; their results are in agreement with those obtained by Winick and Reinhardt [60] using the moment *T*-matrix method.

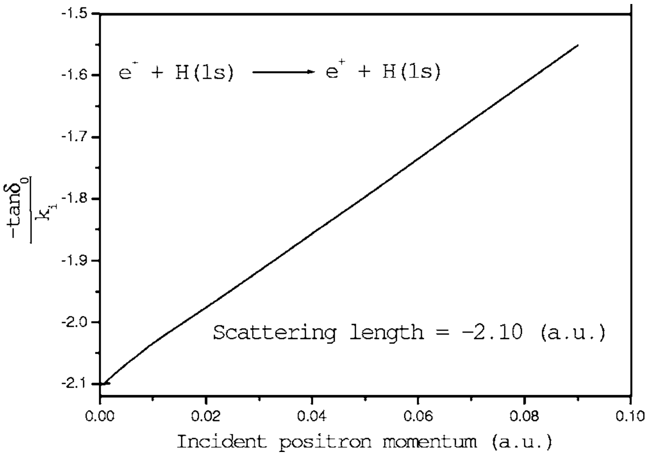

FIG. 1. Scattering length for elastic e^+-H collisions.

We have, however, tested our wave function in these energy regions for all partial waves and have optimized the nonlinear variational parameters to obtain stationary values of the scattering amplitudes. The *S*-wave results are displayed in Table II, whereas the first six partial-wave contributions to the elastic cross sections have been compared in Table III. The agreement of our results in the elastic region (i), the Ore gap region (ii), and last in the most complicated region (iii) establishes satisfactory representation of the scattering mechanism by the present basis set. Besides, we have already shown the ability of our basis set to obtain a converged scattering length. Therefore it is plausible to assume that our basis set is also able to predict satisfactory results for incident positron energies beyond the ionization energy threshold.

C. Positron energy beyond 13.6 eV

The description of positron-hydrogen scattering in this energy region is a formidable proposition for two reasons.

TABLE II. The stationary values of the S-wave elastic scattering amplitudes (a.u.) and phase shifts in e^{+}-H collisions for incident positron energy k_i=0.1–1.0 a.u. along with nonlinear variational parameter p. The numbers within the parentheses indicate the standard deviation in the last figure.

				Phase shifts			
k_i(a.u.)	p	f_L^R	f_L^I	Present results	Kar *et al.* [50]	Bhatia *et al.* [53]	Schwartz [52]
0.10	1.4	0.4390(1)	0.0657(1)	0.1485	0.1482	0.1483	0.151
0.20	1.5	0.5501(1)	0.1045(0)	0.1877	0.1876	0.1877	0.188
0.30	1.6	0.4952(1)	0.0841(0)	0.1682	0.1676	0.1677	0.168
0.40	1.7	0.3589(0)	0.0436(1)	0.1208	0.1200	0.1201	0.120
0.50	1.7	0.2028(1)	0.0138(0)	0.0678	0.0622	0.0624	0.062
0.60	1.8	0.0229(1)	0.0002(2)	0.0076	0.0037	0.0039	0.007
0.70	1.8	−0.1617(1)	0.0087(1)	−0.0540	−0.0515	−0.0512	−0.054
						Chan and Fraser [55]	Humberston [57]
0.71	1.8	−0.1916(1)	0.0123(0)	−0.0641	−0.0580	−0.057	−0.058
0.75	1.8	−0.2478(1)	0.0206(0)	−0.0830	−0.0761	−0.085	−0.076
0.80	1.8	−0.3306(1)	0.0369(0)	−0.1111	−0.1021	−0.110	−0.102
0.85	1.8	−0.4058(1)	0.0559(0)	−0.1370	−0.1247	−0.133	−0.125
0.866	1.8	−0.4239(1)	0.0612(0)	−0.1433	−0.1324	−0.140	
0.90	1.8	−0.4781(2)	0.0782(1)	−0.1622	−0.1398		
1.00	2.0	−0.5898(1)	0.1208(1)	−0.2021	−0.1765		

First, it is necessary to have a large square-integrable basis of hydrogen states to provide an adequate description of the positron-hydrogen ionization continuum. Second, a genuine particle transfer process, namely, positronium formation, also possible. The possibility of positronium formation makes it necessary to include two different manifolds of basis sets, the positron-hydrogen channels and the positronium-proton channels, in the approximation. Thus the conventional variational and other approximate calculations become increasingly complicated and convergence becomes slow. This makes the situation in this energy region rather difficult and there has been a scarcity of calculations which are expected to give a realistic description of the elastic positron-hydrogen scattering. Then if in the trial function of variational methods the effects of the essential desirable factors of the scattering process are included, a realistic description of the scattering problem can hopefully be achieved. The flexibility of the present wave function lies in its capacity to take proper account of the dynamics of the collision problem at the energies considered.

1. S-, P-, and D-wave phase shifts

Tables IV and V include the S-, P-, and D-wave phase shifts obtained by our present calculation. For S waves the effect of distortion decreases monotonically with the increase in energy and disappears at the incident positron momentum of 2.6 a.u. whereas the effect of correlation increases first to attain its maximum at 0.5 a.u. of incident positron momentum and then starts decreasing monotonically to become zero at 1.2 a.u. of incident momentum. For P waves the effect of distortion is nil at very low energy; it then gradually increases and falls down, while the correlation has a very small amount of contribution at very low energy, but like distortion it then gradually rises up and falls down.

The case of D waves is very similar to that of P waves but the effects of both distortion and correlation shift toward higher energy. In Fig. 2 we have plotted S-, P-, and D-wave phase shifts as a function of incident positron momenta. This figure presents three smooth curves of nearly the same nature.

2. F-, G-, H-, and higher-partial-wave phase shifts

Tables IV and V include the results for l=3, 4, 5, 6 partial-wave phase shifts. The scenario for the effects of distortion and correlation for F and G waves is the same as for the D waves, but for H and higher partial waves only static and polarization potentials are enough to produce accurate phase shifts. Figure 3 displays the graphs of F-, G-, and H-wave phase shifts as a function of incident positron momenta. The nature is almost identical to those of the S-, P-, and D-wave graphs.

D. Total elastic cross sections

In this section, we compare in Fig. 4 the total elastic cross section as obtained by the present calculation (as recorded in Tables IV and V) with the 33-state coupled-channel calculation of Kernoghan *et al.* [70] and convergent close-coupling approximation of Bray and Stelbovics [71] in the incident energy range 1–120 eV. It has already been found (Table III) that the partial-wave contributions to the total elastic cross section predicted by us are in conformity with those of

TABLE III. Present partial-wave contributons to the elastic cross section in e^+-H collisions for incident positron momenta 0.1–1.0 a.u.

				l			
k_i(a.u.)	0	1	2	3	4	5	$\Sigma\sigma_L$
0.1	8.7558[a]	0.0897[a]	0.0036[a]	0.0006[a]	0.0001[a]		8.8498
	8.7328[b]	0.0942[b]	0.0035[b]	0.0005[b]	0.0001[b]		
	8.6279[c]	0.0944[c]	0.0037[c]	0.0006[c]	0.0002[c]		
	8.7328[d]	0.0929[e]	0.0034[e]	0.0006[e]	0.0001[e]		
0.2	3.4836[a]	0.3331[a]	0.0142[a]	0.0023[a]	0.0006[a]	0.0002[a]	3.8341
	3.4746[b]	0.3207[b]	0.0151[b]	0.0022[b]	0.0006[b]	0.0002[b]	
	3.4490[c]	0.3207[c]	0.0151[c]	0.0023[c]	0.0006[c]	0.0002[c]	
	3.4819[d]	0.3426[d]	0.0147[e]	0.0022[e]	0.0006[e]	0.0002[e]	
0.3	1.2457[a]	0.5703[a]	0.0301[a]	0.0051[a]	0.0013[a]	0.0005[a]	1.8533
	1.2280[b]	0.5747[b]	0.0370[b]	0.0051[b]	0.0013[b]	0.0004[b]	
	1.2237[c]	0.5747[c]	0.0370[c]	0.0052[c]	0.0013[c]	0.0005[c]	
	1.2382[d]	0.5888[d]	0.0352[e]	0.0051[e]	0.0014[e]	0.0005[e]	
0.4	0.3631[a]	0.7629[a]	0.0699[a]	0.0089[a]	0.0024[a]	0.0008[a]	1.2087
	0.3553[b]	0.7505[b]	0.0726[b]	0.0098[b]	0.0024[b]	0.0008[b]	
	0.3529[c]	0.7505[c]	0.0732[c]	0.0100[c]	0.0024[c]	0.0008[c]	
	0.3589[d]	0.7715[d]	0.0689[e]	0.0088[e]	0.0023[e]	0.0009[e]	
0.5	0.0735[a]	0.8095[a]	0.1186[a]	0.0144[a]	0.0037[a]	0.0013[a]	1.0220
	0.0614[b]	0.8128[b]	0.1254[b]	0.0175[b]	0.0040[b]	0.0013[b]	
	0.0616[c]	0.8141[c]	0.1260[c]	0.0178[c]	0.0040[c]	0.0014[c]	
	0.0622[d]	0.8178[d]	0.1165[e]	0.0198[e]	0.0037[e]	0.0013[e]	
0.6	0.0006[a]	0.7764[a]	0.1950[a]	0.0203[a]	0.0053[a]	0.0019[a]	1.0010
	0.0001[b]	0.7884[b]	0.1978[b]	0.0302[b]	0.0064[b]	0.0020[b]	
	0.0001[c]	0.7863[c]	0.1984[c]	0.0305[c]	0.0065[c]	0.0021[c]	
	0.0002[d]	0.7914[d]	0.1948[e]	0.0202[e]	0.0056[e]	0.0019[e]	
0.7	0.0238[a]	0.7657[a]	0.3038[a]	0.0274[a]	0.0070[a]	0.0025[a]	1.1323
	0.0220[b]	0.7695[b]	0.3174[b]	0.0531[b]	0.0104[b]	0.0030[b]	
	0.0219[c]	0.7746[c]	0.3188[c]	0.0538[c]	0.0108[c]	0.0031[c]	
	0.0214[d]	0.7841[d]	0.3079[e]	0.0272[e]	0.0072[e]	0.0026[e]	
0.8	0.0768[a]	0.6258[a]	0.4217[a]	0.1107[a]	0.0198[a]	0.0033[a]	1.2608
	0.0650[f]	0.5579[f]	0.4226[f]	0.2032[f]	0.0155[f]	0.0037[f]	
	0.065[g]	0.558[h]	0.423[i]	0.200[j]	0.0153[j]	0.0034[j]	
	0.0653[k]	0.626[k]	0.483[k]	0.110[k]	0.0198[k]		
	0.0657[l]	0.626[l]	0.484[l]	0.111[l]			
0.9	0.1288[a]	0.3324[a]	0.4270[a]	0.0960[a]	0.0274[a]	0.0041[a]	1.0190
	0.0958[f]	0.4249[f]	0.4774[f]	0.1338[f]	0.0233[f]	0.0066[f]	
	0.093[j]	0.420[j]	0.472[j]	0.133[j]	0.0221[j]	0.0061[j]	
1.0	0.1611[a]	0.1043[a]	0.3685[a]	0.0795[a]	0.0281[a]	0.0049[a]	0.7507
	0.1231[f]	0.2972[f]	0.3959[f]	0.1447[f]	0.0395[f]	0.0138[f]	
	0.117[j]	0.295[j]	0.394[j]	0.145[j]	0.0396[j]	0.0133[j]	

[a] Present results.

[b] Kuang and Gien [68].

[c] Mitroy [59].

[d] Bhatia *et al.* [53,54].

[e] Roy and Mandal [49].

[f] Kar and Mandal [50].

[g] Humberston [57].

[h] Brown and Humberston [58].

[i] Brown and Humberston [58].

[j] Winick and Reinhardt [60].

[k] Gien [69].

[l] Mitroy [59].

TABLE IV. The Schwinger partial-wave phase shifts δ_l (in radians) in elastic positron-hydrogen collisions for positron momenta 0.1–1.7 a.u.. $x[-y]$ means $x\times 10^{-y}$. Here $\sigma(L)$ denotes the total elastic cross section from L partial-wave contributions, and β, γ are the non linear variational parameters.

k_i	δ_0 β γ	δ_1 β γ	δ_2 β γ	δ_3 β γ	δ_4 β γ	δ_5 β γ	δ_6 β γ	$\sigma(L)$
0.1	0.1485	0.0086	0.0013	0.448[−3]	0.203[−3]	0.108[−3]	0.650[−4]	8.8498(6)
	0.4380	0.0	0.0	0.0	0.0	0.0	0.0	
	0.0331	0.0011	0.0	0.0	0.0	0.0	0.0	
0.2	0.1877	0.0333	0.0053	0.179[−2]	0.813[−3]	0.435[−3]	0.260[−3]	3.8341(7)
	0.4163	0.0	0.0	0.0	0.0	0.0	0.0	
	0.0587	0.0132	0.0	0.0	0.0	0.0	0.0	
0.3	0.1682	0.0654	0.0116	0.401[−2]	0.183[−2]	0.980[−3]	0.585[−3]	1.8533(8)
	0.4002	0.0	0.0	0.0	0.0	0.0	0.0	
	0.0773	0.0376	0.0	0.0	0.0	0.0	0.0	
0.4	0.1208	0.1010	0.0237	0.711[−2]	0.325[−2]	0.174[−2]	0.104[−2]	1.2087(9)
	0.3955	0.0	0.0	0.0	0.0	0.0	0.0	
	0.0840	0.0812	0.0140	0.0	0.0	0.0	0.0	
0.5	0.0678	0.1302	0.0385	0.113[−1]	0.507[−2]	0.272[−2]	0.162[−2]	1.0220(9)
	0.3863	0.0	0.0	0.0	0.0	0.0	0.0	
	0.0900	0.1334	0.0364	0.0019	0.0	0.0	0.0	
0.6	0.0076	0.1532	0.0593	0.161[−1]	0.726[−2]	0.392[−2]	0.234[−2]	1.0001(10)
	0.3733	0.0	0.0	0.0	0.0	0.0	0.0	
	0.0819	0.1944	0.0870	0.0042	0.0	0.0	0.0	
0.7	−0.0540	0.1778	0.0864	0.219[−1]	0.976[−2]	0.532[−2]	0.318[−2]	1.1323(11)
	0.3655	0.1161	0.0	0.0	0.0	0.0	0.0	
	0.0604	0.3121	0.1880	0.0100	0.0	0.0	0.0	
0.8	−0.1111	0.1837	0.1164	0.503[−1]	0.187[−1]	0.691[−2]	0.415[−2]	1.2608(11)
	0.3466	0.2336	0.0	0.0	0.0	0.0	0.0	
	0.0402	0.3874	0.3795	0.1558	0.0433	0.0	0.0	
0.9	−0.1622	0.1504	0.1319	0.527[−1]	0.248[−1]	0.865[−2]	0.534[−2]	1.0190(11)
	0.3289	0.3078	0.0	0.0	0.0	0.0	0.0	
	0.0201	0.2652	0.5561	0.1394	0.0655	0.0	0.0	
1.0	−0.2021	0.0934	0.1362	0.532[−1]	0.280[−1]	0.105[−1]	0.653[−2]	0.7507(12)
	0.3094	1.5258	0.0	0.0	0.0	0.0	0.0	
	0.0125	0.0	0.5681	0.1172	0.0690	0.0	0.0	
1.1	−0.2402	0.0555	0.1318	0.520[−1]	0.307[−1]	0.124[−1]	0.781[−2]	0.6043(12)
	0.2733	0.8512	0.0	0.0	0.0	0.0	0.0	
	0.0054	0.0	0.4836	0.0915	0.0688	0.0	0.0	
1.2	−0.2712	0.0235	0.1013	0.510[−1]	0.320[−1]	0.143[−1]	0.924[−2]	0.4348(13)
	0.2485	0.5332	0.1331	0.1017	0.0	0.0	0.0	
	0.0	0.0	0.2341	0.0711	0.0605	0.0	0.0	
1.3	−0.2971	0.0016	0.0762	0.503[−1]	0.331[−1]	0.161[−1]	0.105[−1]	0.3508(13)
	0.2192	0.4077	0.3331	0.3315	0.1246	0.0	0.0	
	0.0	0.0	0.0688	0.0525	0.0518	0.0	0.0	
1.4	−0.3201	−0.0191	0.0478	0.486[−1]	0.327[−1]	0.178[−1]	0.119[−1]	0.2960(13)
	0.1874	0.2991	0.7124	0.5242	0.3472	0.0	0.0	
	0.0	0.0	0.0	0.0225	0.0323	0.0	0.0	
1.5	−0.3401	−0.0457	0.0340	0.448[−1]	0.323[−1]	0.194[−1]	0.133[−1]	0.2774(14)
	0.1552	0.0	0.3451	1.2438	0.6312	0.0	0.0	
	0.0	0.0	0.0	0.0	0.0070	0.0	0.0	

TABLE IV. (*Continued.*)

k_i	δ_0 β γ	δ_1 β γ	δ_2 β γ	δ_3 β γ	δ_4 β γ	δ_5 β γ	δ_6 β γ	$\sigma(L)$
1.6	–0.3542	–0.0586	0.0235	0.386[–1]	0.318[–1]	0.207[–1]	0.146[–1]	0.2559(14)
	0.1430	0.0	0.1121	0.5857	1.1012	0.0	0.0	
	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
1.7	–0.3650	–0.0706	0.0162	0.345[–1]	0.311[–1]	0.218[–1]	0.158[–1]	0.2405(15)
	0.1378	0.0	0.0	0.3275	0.7017	0.0	0.0	
	0.0	0.0	0.0	0.0	0.0	0.0	0.0	

Kuang and Gien [68], Mitroy [59], Bhatia *et al.* [53,54], Roy and Mandal [49], Kar and Mandal [50], Humberston [57], Brown and Humberston [58], Winick and Reinhardt [60], and Gien [69] in the incident energy range 0.1–1.0 a.u. We have again listed the values of the total elastic cross section in Table VI to compare our results with the Harris-Nesbet algebraic method of Kuang and Gien [68], the 21-state close-coupling calculation of Mitroy [59], the algebraic enlarged six-pseudostate (E6PS) calculation by Gien [69], the Schwinger variational calculation by Roy and Mandal [49] and Kar and Mandal [50], and the five-state close-coupling approximation (CCA) by Basu *et al.* [72] in the incident energy range 0.1–1.0 a.u. It is found that the present results are in accord with all above elaborate calculations.

IV. CONCLUSIONS

Schwinger's variational principle has conveniently and elegantly been used in momentum space to study the elastic positron-hydrogen scattering at low and intermediately energies. Our expression of the scattering amplitude is simple and easy to interpret. In absence of any minimum principle the method uses the stationary property of the scattering amplitude. So the choice of the basis set should be judicious to incorporate the essential physics of the underlying system. Our present investigation uses a discrete basis set which besides having the infinite-order effect of positron-electron correlation duly takes care of the atomic distortion by means of a dipole polarization function. Our findings indicate that for low-energy elastic scattering the effect of the target atom distortion is more than the effect of positron-electron correlation. With the increase in the incident energy as well as in the number of partial waves both these effects gradually decrease. For higher partial-wave contributions inclusion of the static and polarization potentials is sufficient to obtain reliable results.

Finally, it is pertinent to make the point that, with the completion of these studies, it is now possible to safely conclude that the elastic positron-hydrogen collision problem is solved below the ionization threshold for the following reasons.

(a) All the theoretical models predicting definitive results [49,50,52,53,55,57,59,60,68] agree among themselves within a few percent in accuracy in the incident energy range 0–13.6 eV for the first few partial waves.

(b) The Schwinger variational calculations have provided us with equally accurate higher-partial-wave results in this energy range.

(c) All relevant information leading to elastic differen-

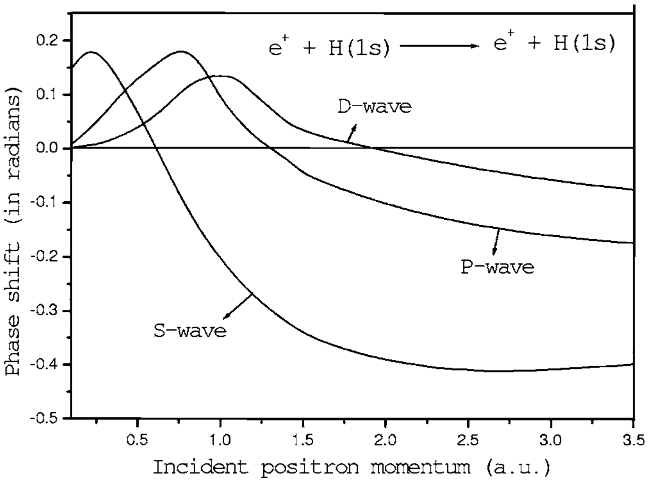

FIG. 2. Display of *S*-, *P*-, and *D*-wave scattering phase shifts in elastic positron-hydrogen collisions for the incident positron momenta 0.1–3.5 a.u.

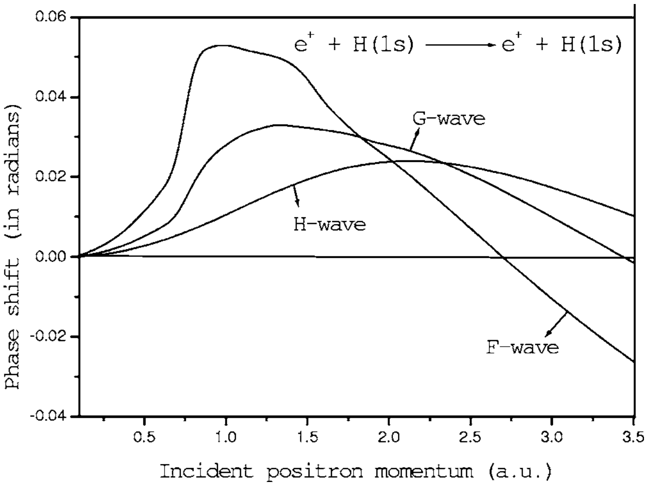

FIG. 3. Display of *F*-, *G*-, and *H*-wave scattering phase shifts in elastic positron-hydrogen collisions for the incident positron momenta 0.1–3.5 a.u.

TABLE V. The Schwinger partial-wave phase shifts δ_l (in radians) in elastic positron-hydrogen collisions for positron momenta 1.8–3.5 a.u.. $x[-y]$ means $x \times 10^{-y}$. Here $\sigma(L)$ denotes the total elastic cross section from L partial-wave contributions, and β, γ are the nonlinear variational parameters.

k_i	δ_0 β γ	δ_1 β γ	δ_2 β γ	δ_3 β γ	δ_4 β γ	δ_5 β γ	δ_6 β γ	$\sigma(L)$
1.8	−0.3751	−0.0818	0.0095	0.307[−1]	0.304[−1]	0.227[−1]	0.169[−1]	0.2276(15)
	0.1249	0.0	0.0	0.1283	0.4841	0.0	0.0	
	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
1.9	−0.3831	−0.0921	0.0029	0.276[−1]	0.287[−1]	0.233[−1]	0.179[−1]	0.2160(15)
	0.1148	0.0	0.0	0.0	0.0	0.0	0.0	
	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
2.0	−0.3902	−0.1016	−0.0037	0.246[−1]	0.279[−1]	0.237[−1]	0.187[−1]	0.2054(15)
	0.1009	0.0	0.0	0.0	0.0	0.0	0.0	
	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
2.1	−0.3953	−0.1102	−0.0101	0.213[−1]	0.269[−1]	0.239[−1]	0.194[−1]	0.1951(16)
	0.0923	0.0	0.0	0.0	0.0	0.0	0.0	
	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
2.2	−0.4002	−0.1182	−0.0163	0.179[−1]	0.256[−1]	0.238[−1]	0.199[−1]	0.1860(16)
	0.0765	0.0	0.0	0.0	0.0	0.0	0.0	
	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
2.3	−0.4052	−0.1254	−0.0223	0.143[−1]	0.241[−1]	0.236[−1]	0.203[−1]	0.1776(16)
	0.0504	0.0	0.0	0.0	0.0	0.0	0.0	
	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
2.4	−0.4071	−0.1321	−0.0280	0.107[−1]	0.224[−1]	0.231[−1]	0.205[−1]	0.1682(16)
	0.0437	0.0	0.0	0.0	0.0	0.0	0.0	
	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
2.5	−0.4082	−0.1381	−0.0336	0.710[−2]	0.205[−1]	0.225[−1]	0.206[−1]	0.1604(17)
	0.0319	0.0	0.0	0.0	0.0	0.0	0.0	
	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
2.6	−0.4114	−0.1435	−0.0389	0.349[−2]	0.185[−1]	0.217[−1]	0.206[−1]	0.1529(17)
	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
2.7	−0.4110	−0.1485	−0.0439	−0.103[−3]	0.164[−1]	0.207[−1]	0.205[−1]	0.1453(17)
	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
2.8	−0.4102	−0.1530	−0.0487	−0.365[−2]	0.143[−1]	0.197[−1]	0.202[−1]	0.1379(17)
	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
2.9	−0.4095	−0.1571	−0.0532	−0.713[−2]	0.121[−1]	0.185[−1]	0.198[−1]	0.1314(18)
	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
3.0	−0.4081	−0.1607	−0.0575	−0.105[−1]	0.988[−2]	0.173[−1]	0.193[−1]	0.1249(18)
	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
3.1	−0.4065	−0.1641	−0.0615	−0.138[−1]	0.762[−2]	0.160[−1]	0.187[−1]	0.1190(18)
	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
3.2	−0.4047	−0.1671	−0.0653	−0.171[−1]	0.534[−2]	0.146[−1]	0.180[−1]	0.1123(18)
	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
	0.0	0.0	0.0	0.0	0.0	0.0	0.0	

TABLE V. (*Continued.*)

k_i	δ_0 β γ	δ_1 β γ	δ_2 β γ	δ_3 β γ	δ_4 β γ	δ_5 β γ	δ_6 β γ	$\sigma(L)$
3.3	−0.4027	−0.1698	−0.0689	−0.202[−1]	0.306[−2]	0.131[−1]	0.173[−1]	0.1084(18)
	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
3.4	−0.4006	−0.1722	−0.0723	−0.232[−1]	0.798[−3]	0.116[−1]	0.165[−1]	0.1068(18)
	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
3.5	−0.3983	−0.1744	−0.0755	−0.262[−1]	−0.144[−2]	0.101[−1]	0.157[−1]	0.099(19)
	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
	0.0	0.0	0.0	0.0	0.0	0.0	0.0	

tial and total cross sections is now available, save the total net reaction cross section including elastic, Ps formation, and excitation cross sections in the energy range 10.2–13.6 eV.

(d) Beyond the positron energy 10.2 eV, however, further definitive calculations are necessary to validate the existing theoretical results before any conclusion can be made.

ACKNOWLEDGMENT

A.G. wishes to thank University Grants Commission (UGC), New Delhi for financial support through a Minor Research Project [Grant No. F. PSW-006/03-04 (ERO)].

APPENDIX: EVALUATION OF TWO-BODY AMPLITUDES FOR ELASTIC POSITRON-HYDROGEN COLLISIONS

In what follows we describe the evaluation of some of the two-body amplitudes as defined in Sec. II in closed analytic form. We have used the basis set (5) to calculate these two-body amplitudes.

For elastic positron-H collisions, we have

$$\phi_i(\vec{r}_2) = N_i \exp(-\lambda_i r_2) \tag{A1}$$

where $N_i = \sqrt{\lambda_i^3/\pi}$, $\lambda_i = 1/a_0 = 1$ a.u., and $f \equiv i$.

1. $A_{nm}(\vec{k}_f,\vec{k}_i)$

The amplitude $A_{nm}(\vec{k}_f,\vec{k}_i)$ is given by

$$A_{nm}(\vec{k}_f,\vec{k}_i) = \left(-\frac{\mu_f}{2\pi}\right)\langle v_n|V_i|u_m\rangle = \left(-\frac{\mu_f}{2\pi}\right)\int v_n * V_i u_m d\vec{r}_1 d\vec{r}_2 \tag{A2}$$

which on using the expressions for v_n^*, u_m, and $V_i = 1/r_1 - 1/r_{12}$ becomes

TABLE VI. Integrated cross sections (πa_0^2) for elastic positron-hydrogen collisions in the incident momenta range 0.1–0.8 a.u.

	k_i(a.u.)							
	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8
Present result	8.8498	3.8341	1.8533	1.2087	1.0220	1.0010	1.1323	1.2608
Harris-Nesbet[a]	8.828	3.815	1.848	1.194	1.025	1.029	1.181	1.308
21-state CCA[b]	8.736	3.787	1.844	1.192	1.026	1.026	1.186	1.316
Algebraic E6PS[c]	8.835	3.818	1.849	1.194	1.023	1.025	1.179	1.311
Variational[d]	8.713	3.802	1.849	1.213	1.030	1.003	1.101	1.2679[e]
Five-state CCA[f]	8.839	3.838	1.866	1.209	1.031	1.020	1.160	1.239

[a] Harris-Nesbet algebraic method; Kuang *et al.* [68].

[b] 21-state close-coupling approach; Mitroy (1995) [59].

[c] Algebraic enlarged six-pseudostate calculation (E6PS); Gien [69].

[d] Schwinger variational principle; Roy and Mandal [49].

[e] Kar and Mandal [50].

[f] Five-state CCA; Basu *et al.* [72].

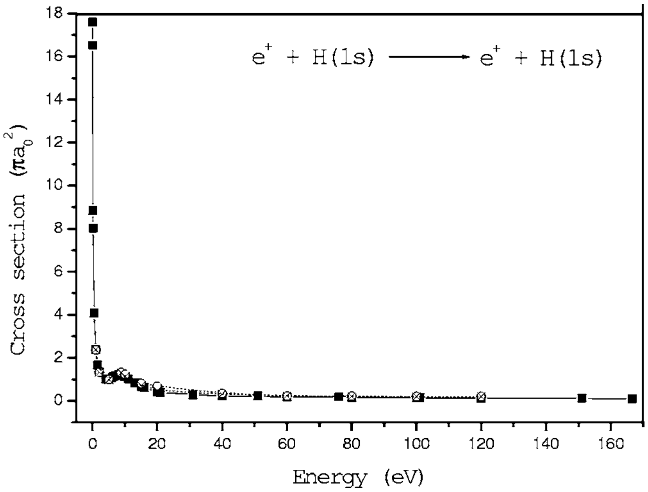

FIG. 4. Integrated cross section (πa_0^2) for elastic scattering of positron by hydrogen atom in the incident energy range 1–167 eV: shaded squares, present Schwinger results; open circles, 33-state results of Kernoghan *et al.* [70]; crosses, convergent close-coupling approximation (Bray and Stelbovics [71]).

$$A_{nm}(\vec{k}_f,\vec{k}_i) = \left(-\frac{\mu_f}{2\pi}\right)|N_i|^2 \times \int e^{i\vec{q}\cdot\vec{r}_1}(1-e^{-pr_1})^2 e^{-b_3 r_2-\gamma_{nm}r_{12}} r_1^{m_0+n_0-2} \times \left(\frac{1}{r_1}-\frac{1}{r_{12}}\right) d\vec{r}_1 d\vec{r}_2, \tag{A3}$$

where $\vec{q}=\vec{k}_i-\vec{k}_f$, $b_3=2\beta+2\lambda_i$, and $\gamma_{nm}=2\gamma$.

To evaluate the above integral (A3) we first evaluate the following type integral:

$$I(\vec{v},a,b,c,n) = \int e^{i\vec{v}\cdot\vec{r}_1-ar_1-br_2-cr_{12}} r_1^n \left(\frac{1}{r_1}-\frac{1}{r_{12}}\right) d\vec{r}_1 d\vec{r}_2 = I_1(\vec{v},a,b,c,n) - I_2(\vec{v},a,b,c,n) \quad \text{(say)}. \tag{A4}$$

Now

$$\begin{aligned} I_1(\vec{v},a,b,c,n) &= \int e^{i\vec{v}\cdot\vec{r}_1-ar_1-br_2-cr_{12}} r_1^n \frac{1}{r_1} d\vec{r}_1 d\vec{r}_2 \\ &= \int e^{i\vec{v}\cdot\vec{r}_1-ar_1} r_1^n \frac{1}{r_1}\left(\int e^{-br_2-cr_{12}} d\vec{r}_2\right) d\vec{r}_1 \\ &= \int e^{i\vec{v}\cdot\vec{r}_1-ar_1} r_1^n \frac{1}{r_1}\frac{4\pi}{(b^2-c^2)^2} \\ &\quad \times\left[\frac{-8bc}{(b^2-c^2)}\left(\frac{e^{-cr_1}}{r_1}-\frac{e^{-br_1}}{r_1}\right) + 2ce^{-br_1}+2be^{-cr_1}\right] d\vec{r}_1, \end{aligned} \tag{A5}$$

where we have taken Fourier integral transforms for functions of the form $\exp(-\lambda r)/r$, $\exp(-\lambda r)$:

$$\exp(-\lambda r)/r = \frac{1}{2\pi^2}\int \frac{e^{i\vec{p}\cdot\vec{r}}}{p^2+\lambda^2} d\vec{p}, \tag{A6}$$

$$\exp(-\lambda r) = \frac{\lambda}{\pi^2}\int \frac{e^{i\vec{p}\cdot\vec{r}}}{(p^2+\lambda^2)^2} d\vec{p} \tag{A7}$$

and utilized the δ-function properties, such as

$$\int e^{i(\vec{q}-\vec{\Delta})\cdot\vec{r}} f(\vec{q}) d\vec{q}\, d\vec{r} = (2\pi)^3 \int \delta(\vec{q}-\vec{\Delta}) f(\vec{q}) d\vec{q} = (2\pi)^3 f(\vec{\Delta}). \tag{A8}$$

Similarly we obtain

$$\begin{aligned} I_2(\vec{v},a,b,c,n) &= \int e^{i\vec{v}\cdot\vec{r}_1-ar_1-br_2-cr_{12}} r_1^n \frac{1}{r_{12}} d\vec{r}_1 d\vec{r}_2 \\ &= \int e^{i\vec{v}\cdot\vec{r}_1-ar_1} r_1^n \left(\int e^{-br_2-cr_{12}}\frac{1}{r_{12}} d\vec{r}_2\right) d\vec{r}_1 \\ &= \int e^{i\vec{v}\cdot\vec{r}_1-ar_1} r_1^n \frac{4\pi}{(b^2-c^2)} \\ &\quad \times\left[\frac{2b}{(b^2-c^2)}\left(\frac{e^{-cr_1}}{r_1}-\frac{e^{-br_1}}{r_1}\right) - e^{-br_1}\right] d\vec{r}_1. \end{aligned} \tag{A9}$$

Substituting integrals (A5) and (A9) in integral (A4), we obtain

$$\begin{aligned} I(\vec{v},a,b,c,n) &= \int e^{i\vec{v}\cdot\vec{r}_1-ar_1} r_1^n \frac{4\pi}{(b^2-c^2)}\left[\frac{-8bc}{(b^2-c^2)^2}\left(\frac{e^{-cr_1}}{r_1^2}\right.\right. \\ &\quad \left.\left.-\frac{e^{-br_1}}{r_1^2}\right) + \frac{2(b+c)}{(b^2-c^2)}\frac{e^{-br_1}}{r_1} + e^{-br_1}\right] d\vec{r}_1. \end{aligned} \tag{A10}$$

In order to bring the integral (A10) in a closed analytical form we now compute the following integral:

$$\begin{aligned} f(\vec{q},\lambda,n) &= \int r^n e^{i\vec{q}\cdot\vec{r}-\lambda r} d\vec{r} \\ &= \frac{4\pi}{q}\int_0^\infty r^{n+1} e^{-\lambda r}\sin qr\, dr \\ &= \frac{4\pi}{q}(-1)^{n+1}\left(\frac{\partial}{\partial\lambda}\right)^{n+1}\int_0^\infty e^{-\lambda r}\sin qr\, dr \\ &= \frac{4\pi}{q}\frac{\Gamma(n+2)}{(\lambda^2+q^2)^{(n+2)/2}}\sin\left((n+2)\tan^{-1}\frac{q}{\lambda}\right). \end{aligned} \tag{A11}$$

Now substituting the closed result of integral (A11) in (A10) we finally have the analytical expression

$$I(\vec{v},a,b,c,n) = \frac{4\pi}{(b^2-c^2)}\left(\frac{-8bc}{(b^2-c^2)^2}[f(\vec{v},a+c,n-2) - f(\vec{v},a+b,n-2)] + \frac{2(b+c)}{(b^2-c^2)}f(\vec{v},a+b,n-1) + f(\vec{v},a+b,n)\right). \tag{A12}$$

Using (A12) we thus obtain $A_{nm}(\vec{k}_f,\vec{k}_i)$ as

$$A_{nm}(\vec{k}_f,\vec{k}_i) = C[I(\vec{q},0,b_3,\gamma_{nm},m_0+n_0-2) - 2I(\vec{q},p,b_3,\gamma_{nm},m_0 + n_0-2) + I(\vec{q},2p,b_3,\gamma_{nm},m_0+n_0-2)] \tag{A13}$$

with $C=(-\mu_f/2\pi)|N_i|^2=-1/2\pi^2$, $\mu_f=1$ a.u.

2. $A_{ni}(\vec{k}_f,\vec{k}_i)$

The amplitude $A_{ni}(\vec{k}_f,\vec{k}_i)$ is given by

$$A_{ni}(\vec{k}_f,\vec{k}_i) = \left(-\frac{\mu_f}{2\pi}\right)\langle v_n|V_i|\Phi_i\rangle = \left(-\frac{\mu_f}{2\pi}\right)\int v_n * V_i\Phi_i d\vec{r}_1 d\vec{r}_2 \tag{A14}$$

which on using the expressions for v_n^*, Φ_i, and $V_i=1/r_1 -1/r_{12}$ becomes

$$A_{ni}(\vec{k}_f,\vec{k}_i) = \left(-\frac{\mu_f}{2\pi}\right)|N_i|^2\int e^{i\vec{q}\cdot\vec{r}_1}(1-e^{-pr_1})e^{-b_2r_2-\gamma r_{12}}r_1^{n_0-1} \times\left(\frac{1}{r_1}-\frac{1}{r_{12}}\right)d\vec{r}_1 d\vec{r}_2 = C[I(\vec{q},0,b_1,\gamma,n_0-1) - I(\vec{q},p,b_1,\gamma,n_0-1)] \tag{A15}$$

with $b_1=\beta+2\lambda_i$.

3. $A_{fm}(\vec{k}_f,\vec{k}_i)$

Similarly the amplitude $A_{fm}(\vec{k}_f,\vec{k}_i)$ is given by

$$A_{fm}(\vec{k}_f,\vec{k}_i) = \left(-\frac{\mu_f}{2\pi}\right)\langle\Phi_f|V_i|u_m\rangle = \left(-\frac{\mu_f}{2\pi}\right)\int \Phi_f^* V_i u_m d\vec{r}_1 d\vec{r}_2 \tag{A16}$$

which on using the expressions for Φ_f^*, u_m, and $V_i=1/r_1 -1/r_{12}$ becomes

$$A_{fm}(\vec{k}_f,\vec{k}_i) = \left(-\frac{\mu_f}{2\pi}\right)|N_i|^2\int e^{i\vec{q}\cdot\vec{r}_1} \times(1-e^{-pr_1})e^{-b_3r_2-\gamma r_{12}}r_1^{m_0-1}\left(\frac{1}{r_1}-\frac{1}{r_{12}}\right)d\vec{r}_1 d\vec{r}_2 = C[I(\vec{q},0,b_2,\gamma,m_0-1) - I(\vec{q},p,b_3,\gamma,m_0-1)] \tag{A17}$$

with $b_3=\beta+2\lambda_i$.

---

[1] L. Hulthen, K. Fysiogr. Saellsk. Lund, Foerh. **14**, 21 (1944); Ark. Mat., Astron. Fys. **35A** 25 (1948).

[2] I. G. Tamm, Zh. Eksp. Teor. Fiz. **14**, 21 (1948); **18**, 337 (1948); **19**, 74 (1949).

[3] J. Schwinger, Phys. Rev. **72**, 742 (1947).

[4] W. Kohn, Phys. Rev. **74**, 1763 (1948).

[5] S. Huang, Phys. Rev. **75**, 980 (1949); **76**, 477 (1949); **76**, 866 (1949); M. Verde, Helv. Phys. Acta **22**, 339 (1949); H. Feshbach and S. I. Rubinow, Phys. Rev. **88**, 484 (1952); H. E. Moses, *ibid.* **92**, 817 (1953); R. E. B. Makinson and J. S. Turner, Proc. Phys. Soc., London, Sect. A **66**, 857 (1953); **66**, 866 (1953); S. I. Rubinow, Phys. Rev. **98**, 183 (1955); M. Moe and D. S. Saxon, *ibid.* **111**, 950 (1958); F. E. Harris, Phys. Rev. Lett. **19**, 173 (1967); J. Nuttall, Ann. Phys. (N.Y.) **52**, 428 (1969).

[6] J. M. Blatt and J. D. Jackson, Phys. Rev. **76**, 18 (1949).

[7] T. Kato, Prog. Theor. Phys. **6**, 195 (1951).

[8] J. M. Blatt and L. C. Biedenharn, Phys. Rev. **86**, 399 (1952); Phys. Rev. **93**, 1387 (1954).

[9] N. F. Mott and H. S. W. Massey, *The Theory of Atomic Collisions* (Oxford University Press, New York, 1965). 3rd ed.

[10] B. L. Moiseiwitsch, *Variational Principles* (Wiley, New York, 1966).

[11] C. J. Joachain, *Quantum Collision Theory* (North-Holland, New York, 1979), pp. 225–242.

[12] P. G. Burke, *Potential Scattering in Atomic Physics* (Plenum, London, 1977).

[13] B. H. Bransden, *Atomic Collision Theory* (Benjamin-Cummins, Reading, MA, 1983), pp. 59–109.

[14] B. W. Schmid and H. Ziegelmann, *The Quantum Mechanical Three-Body Problem* (Pergamon, Oxford, 1974), pp. 163–205

[15] R. K. Nesbet, *Variational Methods in Electron-Atom Scattering Theory* (Plenum, New York, 1980).

[16] R. G. Newton, *Scattering Theory of Waves and Particles* (McGraw-Hill, New York, 1966).

[17] S. Altshuler, Phys. Rev. **89**, 1278 (1953).

[18] C. Schwartz, Phys. Rev. **141**, 1468 (1966).

[19] M. A. Abdel-Raouf, Phys. Rep. **108**, 1 (1984).

[20] H. E. Saraph, Proc. Phys. Soc. London **77**, 827 (1961).

[21] T. L. John, Proc. Phys. Soc. London **76**, 532 (1960).

[22] R. R. Lucchese and V. McKoy, Phys. Rev. A **28**, 1382 (1983).

[23] D. K. Watson and V. McKoy, Phys. Rev. A **20**, 1474 (1979).

[24] R. R. Lucchese, D. K. Watson, and V. McKoy, Phys. Rev. A **22**, 421 (1980).

[25] R. R. Lucchese, K. Takatsuka, and V. McKoy, Phys. Rep. **131**, 147 (1986).

[26] K. Takatsuka and V. McKoy, Phys. Rev. A **23**, 2352 (1981).

[27] K. Takatsuka and V. McKoy, Phys. Rev. Lett. **45**, 1396 (1980); **24**, 2473 (1981); **23**, 2352 (1981).

[28] K. Takatsuka and V. McKoy, Phys. Rev. A **24**, 2473 (1981).

[29] H. P. Pritchard, M. A. P. Lima, and V. McKoy, Phys. Rev. A **39**, 2392 (1989).

[30] F. E. Harris and H. H. Michels, Methods Comput. Phys. **10**, 143 (1971); Phys. Rev. Lett. **22**, 1036 (1969).

[31] R. K. Nesbet and R. S. Oberoi, Adv. Quantum Chem. **9**, 215 (1975); Adv. At. Mol. Phys. **13**, 315 (1977).

[32] I. H. Sloan and S. K. Adhikari, Nucl. Phys. A **235**, 352 (1974); **241**, 429 (1975).

[33] A. L. Zubarev, Sov. Phys. J. **29**, 281 (1979); Sov. J. Part. Nucl. **7**, 215 (1976).

[34] V. B. Balayev, A. P. Podkopayev, J. Wrzeionko, and A. L. Zubarev, J. Phys. B **12**, 1225 (1979).

[35] J. Nuttal, in *The Padé Approximant in Theoretical Physics*, edited by George A Baker, Jr., and J. L. Gammel (Academic, New York, 1970), p. 219.

[36] C. Schwartz and C. Zemach, Phys. Rev. **141**, 1454 (1966).

[37] N. Maleki, Ph.D. thesis, University of Nebraska, 1981 (unpublished).

[38] N. Maleki and J. Macek, Phys. Rev. A **21**, 1403 (1980).

[39] S. K. Adhikari, Phys. Rev. A **42**, 6 (1990).

[40] Y. Hahn, Phys. Rev. A **26**, 808 (1982).

[41] W. Domcke, J. Phys. B **12**, 2675 (1982).

[42] D. K. Watson, Phys. Rev. A **29**, 558 (1984); **34**, 1016 (1986); J. Phys. B **19**, 293 (1986).

[43] K. Takatsuka and V. McKoy, Phys. Rev. A **23**, 2359 (1981).

[44] R. Sugar and R. Blankenbecler, Phys. Rev. **136B**, 472 (1964).

[45] B. L. Moiseiwitsch, J. Phys. B **15**, L609 (1982); **15**, L863 (1982); Proc. Phys. Soc. London **72**, 139 (1958).

[46] R. S. Singh and A. D. Stauffer, Nuovo Cimento Soc. Ital. Fis., B **25**, 547 (1975).

[47] A. L. Zubarev, Theor. Math. Phys. **30**, 45 (1977).

[48] B. I. Schneider and L. A. Collins, Phys. Rev. B **136B**, 472 (1981); J. Phys. B **14**, L101 (1981).

[49] U. Roy and P. Mandal, J. Phys. B **22**, L261 (1989); **23**, L55 (1990); Phys. Rev. A **48**, 2952 (1993); **48**, 2952 (1993).

[50] S. Kar and P. Mandal, J. Phys. B **30**, L627 (1997).

[51] S. Kar and P. Mandal, J. Phys. B **32**, 2297 (1999); Phys. Rev. A **59**, 1913 (1999); J. Phys. B **33**, L165 (2000); Phys. Rev. A **62**, 052514 (2000).

[52] C. Schwartz, Phys. Rev. **124**, 1468 (1961).

[53] A. K. Bhatia, A. Temkin, R. J. Drachman, and H. Eiserike, Phys. Rev. A **3**, 1328 (1971).

[54] A. K. Bhatia, A. Temkin, and H. Eiserike, Phys. Rev. A **9**, 219 (1974).

[55] Y. F. Chan and P. A. Fraser, J. Phys. B **6**, 2504 (1973).

[56] Y. F. Chan and R. P. McEachran, J. Phys. B **9**, 2869 (1976).

[57] J. W. Humberston, J. Phys. B **17**, 2353 (1984).

[58] C. J. Brown and J. W. Humberston, J. Phys. B **17**, L423 (1984); **18**, L401 (1985).

[59] J. Mitroy, J. Phys. B **29**, L263 (1996); Aust. J. Phys. **48**, 645 (1995); **48**, 893 (1995).

[60] J. R. Winick and W. P. Reinhardt, Phys. Rev. A **18**, 925 (1978).

[61] R. Damburg and E. Karule, Proc. Phys. Soc. London **90**, 637 (1967).

[62] R. M. Sternheimer, Phys. Rev. **96**, 951 (1954).

[63] A. Temkin and J. C. Lamkin, Phys. Rev. **121**, 788 (1961).

[64] S. K. Houston and R. J. Drachman, Phys. Rev. A **3**, 1335 (1971).

[65] J. W. Humberston and J. B. Wallace, J. Phys. B **5**, 1138 (1972).

[66] C. J. Keinman, Y. Hahn, and L. Spruch, Phys. Rev. **140A**, 413 (1965).

[67] R. L. Armstead, Phys. Rev. **171**, 91 (1968).

[68] Y. R. Kuang and T. T. Gien, Phys. Rev. A **55**, 256 (1997).

[69] T. T. Gien, J. Phys. B **30**, L23 (1997).

[70] A. A. Kernoghan, D. J. R. Robinson, M. T. McAlinden, and H. R. J. Walters, J. Phys. B **29**, 2089 (1996).

[71] I. Bray and A. T. Stelbovics, Phys. Rev. A **49**, R2224 (1994).

[72] M. Basu, M. Mukherjee, and A. S. Ghosh, J. Phys. B **23**, 1 (1990).