Multichannel Schwinger's principle for rearrangement collisions: Positronium formation in positron-hydrogen collisions

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Post and prior forms of the multichannel Schwinger's principle for rearrangement collisions are presented using discrete basis sets. An application is made to positronium formation in positron-hydrogen collisions at low energies in the range 6.8–30.0 eV. A total number of eight terms of a type of correlated basis functions involving inverse powers of half-odd integers is required to predict accurate results in conformity with the available variational and nonvariational values in the literature. Our findings indicate that destructive interference between partial-wave contributions to the scattering amplitude is responsible for the appearance of critical angles in positronium formation. Surface plots of the differential cross section display immensely rich structure. The total positronium formation cross sections agree nicely with the observed data of Zhou *et al.* [Phys. Rev. A **55**, 361 (1997)] in the entire energy range. [S1050-2947(99)01802-8]

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I. INTRODUCTION

It is nearly two decades since Schwinger's variational principle was proposed to be used with renewed interest to study electron-atom and electron-molecule collisions by McKoy and co-workers with discrete basis set expansions [1–5]. Applications of the method in momentum space have been made for positron-atom collisions using correlated basis sets [6,7]. Definitive results for three-body nuclear reactions have also been reported in the literature [8].

In this paper, we present a formulation of Schwinger's variational principle in the discrete basis set expansion for rearrangement collisions [9,10] such as

$$1+(2,3)\rightarrow(1,2)+3. \tag{1}$$

One of the virtues of this method is that, as for direct collisions, it is not required to know the asymptotic behavior of the scattering wave function; this is taken care of by the Green's function involved in the variational principle. Furthermore, the present method in momentum space is readily applicable to higher partial waves in a straightforward manner, unlike formulations in configuration space, in which an evaluation of the so-called second-order terms $\langle\Phi_f|V_f G_f^+ V_i|\Phi_i\rangle$ or $\langle\Phi_f|V_f G_i^+ V_i|\Phi_i\rangle$ becomes enormously difficult. As we shall see, in our formulation, the evaluation of these matrix elements is conveniently transformed into a principal value integral in one dimension in the k plane; we have a well-tested prescription for its numerical calculation.

We make an application of the above formalism to positronium (Ps) formation in positron-hydrogen collisions, which is a rather complicated rearrangement collision process in a perfect three-body scattering system: $e^+ + (e^-,p) \rightarrow (e^+,e^-) + p$. Since the pioneering work of Massey and Mohr in 1954 [11], this process has been studied by a variety of methods with various degrees of sophistication [6,12–21]. Among these, accurate Kohn-Hulthĕn variational results for a few partial waves, $L=0$, 1, and 2, at incident energies in the Oré gap, (6.8–10.2 eV) have been reported by Stein and Sternlicht [12], Humberston [13(a)], and Brown and Humberston [13(b)]. Recently Gien [14] reported a Harris-Nesbet variational calculation in close agreement with those calculations. At these energies, reasonably accurate values of the K matrix have also been reported by a preliminary calculation of the Schwinger principle [6]. For intermediate and higher energies of positron impact, particular mention may be made of calculations using the impulse approximation [15], the distorted-wave approximations [16,17], Fock-Tani field-theoretic equations [18], the R-matrix method [19], the coupled 33-state method [20] and the 28-state close-coupling approximation method [21].

Remarkable experiments were recently reported for total Ps formation and total reaction cross sections in Refs. [22] and [23]. The observed data are in accord with theoretical predictions in the overall shape and nature of the cross section, but differ significantly in one way or the other in details. However progress has been noteworthy and quite encouraging in that broad areas of disagreement are gradually being narrowed down and their causes being analyzed with purpose and devotion as the nature of the problem so demands.

One of the interesting features of our calculation is that only eight terms of a new correlated basis function involving inverse powers of half-odd integers are required to predict accurate amplitudes and cross sections for partial waves $L=0-15$, at positron energies in the range 6.8–30.0 eV. These results are in accord with Kohn-Hulthĕn and Harris-Nesbet variational calculations available in the literature [13,14]. Critical angles are predicted in Ps formation, and are displayed through surface plots of the differential cross sections.

The plan of the paper is as follows. In Sec. II we present the formulation of Schwinger's principle for rearrangement collisions using discrete basis sets. Section III describes the application of the ''prior'' form of the amplitudes to Ps formation in positron-hydrogen collisions. The forms of two-body amplitudes required for a determination of the stationary Schwinger amplitude with the use of correlated basis

functions are given in this section, and their methods of evaluation suggested. Results of our calculation are presented in Sec. IV. Finally, concluding remarks are made in Sec. V. Atomic units are used in the present work.

II. THEORY

Let us consider a three-body scattering system in which particle 1 with mass m_1 is incident on a bound system of particles 2 and 3 with masses m_2 and m_3, respectively, in the initial channel. In the final rearrangement channel, particles 1 and 2 form a bound pair, while particle 3 remains a spectator. Let V_1 denote the interaction between particles 2 and 3, V_2 the interaction between particles 1 and 3, and V_3 the interaction between particles 1 and 2. The total interaction in the scattering is $V=V_1+V_2+V_3$, while the residual interactions in the incident and the final channels are $V_i=V_2+V_3$ and $V_f=V_1+V_2$, respectively.

If H denotes the full Hamiltonian of the scattering system, it can be expressed in terms of the channel Hamiltonians as

$$H=H_i+V_i=H_f+V_f, \tag{2}$$

such that

$$H_i\Phi_i=E_i\Phi_i, \quad H_f\Phi_f=E_f\Phi_f. \tag{3}$$

Energy conservation requires that, on the energy shell, $E_i=E_f=E$, the total energy of the system. The Green's operators are defined as

$$G_i^{\pm}=\frac{1}{E-H_i\pm i\epsilon}, \quad G_f^{\pm}=\frac{1}{E-H_f\pm i\epsilon}, \quad G^{\pm}=\frac{1}{E-H\pm i\epsilon}. \tag{4}$$

Using the operator relations $(1/A)-(1/B)=(1/A)(B-A)\times(1/B)=(1/B)(B-A)(1/A)$, the integral equations for the total Green's operators $G^{\pm}$ may be obtained as

$$G^{\pm}=G_i^{\pm}+G_i^{\pm}V_iG^{\pm}=G_i^{+}+G^{\pm}V_iG_i^{\pm}, \tag{5a}$$

$$G^{\pm}=G_f^{\pm}+G_f^{\pm}V_fG^{\pm}=G_f^{+}+G^{\pm}V_fG_f^{\pm}. \tag{5b}$$

It can be easily verified that the full scattering wave functions Ψ_i^{+} and Ψ_f^{-} for the incident and final channels satisfy the Lippmann-Schwinger integral equations:

$$\Psi_i^{\pm}=\Omega_i^{\pm}\Phi_i=\Phi_i+G_i^{\pm}V_i\Psi_i^{\pm} =\Phi_i+G_i^{\pm}V_i\Phi_i+G_i^{\pm}V_iG_i^{\pm}V_i\Phi_i+\cdots, \tag{6a}$$

$$\Psi_f^{\pm}=\Omega_f^{\pm}\Phi_f=\Phi_f+G_f^{\pm}V_f\Psi_f^{\pm} =\Phi_f+G_f^{\pm}V_f\Phi_f+G_f^{\pm}V_fG_f^{\pm}V_f\Phi_f+\cdots. \tag{6b}$$

where the Møller operators are defined as

$$\Omega_i^{\pm}=1+G^{\pm}V_i, \tag{7a}$$

$$\Omega_f^{\pm}=1+G^{\pm}V_f. \tag{7b}$$

The post and prior forms of the Born series for transition from the bound state i in the initial channel α to the state f in the final channel β may now be defined, on the energy shell, as

$$T_{fi}^{(\mathrm{prior})}(\beta\vec{k}_f,\alpha\vec{k}_i)=\langle\Phi_f|V_f|\Psi_i^{+}\rangle =\langle\Phi_f|V_f(\mathrm{or}\,V_i)+V_fG_i^{+}V_i+V_fG_i^{+}V_iG_i^{+}V_i +\cdots|\Phi_i\rangle, \tag{8a}$$

$$T_{fi}^{(\mathrm{post})}(\beta\vec{k}_f,\alpha\vec{k}_i)=\langle\Psi_f^{-}|V_i|\Phi_i\rangle =\langle\Phi_f|V_i(\mathrm{or}\,V_f)+V_fG_f^{+}V_i+V_fG_f^{+}V_fG_f^{+}V_i +\cdots|\Phi_i\rangle, \tag{8b}$$

where $\hbar\vec{k}_i$ and $\hbar\vec{k}_f$ denote, respectively, the momenta of the center-of-mass motion in the incident and final channels. As is well known, retaining the first two terms of the above series would yield the first and second Born terms of the transition matrix as

$$T_I^{(\mathrm{post})}(\beta\vec{k}_f,\alpha\vec{k}_i)=\langle\Phi_f|V_f|\Phi_i\rangle, \tag{9a}$$

$$T_I^{(\mathrm{prior})}(\beta\vec{k}_f,\alpha\vec{k}_i)=\langle\Phi_f|V_i|\Phi_i\rangle, \tag{9b}$$

$$T_{II}^{(\mathrm{post})}(\beta\vec{k}_f,\alpha\vec{k}_i)=\langle\Phi_f|V_fG_f^{+}V_i|\Phi_i\rangle, \tag{10a}$$

$$T_{II}^{(\mathrm{prior})}(\beta\vec{k}_f,\alpha\vec{k}_i)=\langle\Phi_f|V_fG_i^{+}V_i|\Phi_i\rangle. \tag{10b}$$

If the bound states in the plane waves Φ_i and Φ_f are known exactly, the post and prior forms of the first Born matrix element [Eqs. (9a) and (9b)] would give identical results. If, however, the bound states are supposed to be inexactly known, as for composite particles, there would arise what is known as the ''post-prior'' discrepancy between the two matrix elements. For the second-order Born terms of Eqs. (10a) and (10b), the contributions made by the two forms are not generally equal, so long as G_i^{+} and G_f^{-} as well as V_i and V_f are different. A large number of applications has been made with the prior form of the second Born approximation to rearrangement collisions in atomic and molecular collisions, but the post form has rarely been utilized and its usefulness is relatively unknown so far.

The importance of the second-order terms in the study of rearrangement collisions has nevertheless been acknowledged for a long time. In order to describe the charge transfer in ion-atom collisions, such as $Z_B+(e,Z_A)\rightarrow(e,Z_B)+Z_A$, Thomas [24] proposed that the reaction takes place as a two-step process. In the first step, the incoming ion on its trajectory of motion knocks the electron toward its parent nucleus. The electron is elastically scattered, in the second step, by the nucleus along the direction of the projectile. While the center of mass of the (electron, projectile) bound pair moves away from it, the atomic nucleus remains a mere spectator. This classical model has been successfully applied to analyze charge-transfer collisions, and has been gainfully employed in the understanding and analysis of the quantum-mechanical prescriptions [25,26].

It is, however, clear that the use of the Born series for the study of rearrangement collisions is not quite adequate for

various reasons. For low energies of projectile impact, it is desired that the distortion of the atomic and molecular charge cloud due to the slowly moving projectile's charge be described properly with a consideration of distorted atomic or molecular orbitals rather than using plane waves for them as in the Born approximation. The question of convergence of the Born series has been investigated by several authors. Dettman and Leibfried [27] showed that, at high energies, the first two terms of the Born series of the T-matrix element for nonrelativistic rearrangement collisions occurring in a three-body system give the correct energy dependence [25,26].

One of the higher-order methods that naturally reduces to the second Born approximation under certain restrictions is the Schwinger variational principle. Following Joachain [9,10], we obtain a convenient expression of the scattering amplitude for rearrangement collisions using discrete basis sets. The transition operator for the purpose is defined as $\tau_{fi}=V_f\Omega_i^+$, and, on using the following property of the Møller operators: $V_f[\Omega_f^+-1]=[\Omega_f^--1]^\dagger V_i$, one obtains the expression $\tau_{fi}=(\Omega_f^-)^\dagger V_i+V_f-V_i$. It is now possible to define a pair of variational principles for the transition operator τ_{fi}:

$$[R_1]=(\Omega_f^-)^\dagger V_f G_f^+ V_i+V_f\Omega_i^+-(\Omega_f^-)^\dagger[V_f-V_f G_f^+ V_f]\times(\Omega_i^+-1), \tag{11a}$$

$$[R_2]=V_f G_i^+ V_i\Omega_i^+ +(\Omega_f^-)^\dagger V_i+V_f-V_i-(\Omega_f^--1)^\dagger\times[V_i-V_i G_i^+ V_i]\Omega_i^+ . \tag{11b}$$

Indeed, it can be shown that $[R_1]=\tau_{ij}=[R_2]$ and that these expressions are stationary for independent variations of the Møller operators about their correct values: $\delta[R_1]=0=\delta[R_2]$. When the matrix elements of these stationary expressions $[R_1]$ and $[R_2]$ are taken between free states Φ_i and Φ_f, one obtains the post and prior forms of the stationary transition matrix elements respectively as [9,10]

$$[T_{fi}(\beta\vec{k}_f,\alpha\vec{k}_i)]_{\rm post}=\langle\Phi_f|V_f|\Psi_i^+\rangle+\langle\Psi_f^-|V_f+V_f G_f^+(V_i-V_f)|\Phi_i\rangle-\langle\Psi_f^-|V_f-V_f G_f^+ V_f|\Psi_i^+\rangle, \tag{12a}$$

$$[T_{fi}(\beta\vec{k}_f,\alpha\vec{k}_i)]_{\rm prior}=\langle\Phi_f|V_i+(V_f-V_i)G_i^+ V_i|\Psi_i^+\rangle+\langle\Psi_f^-|V_i|\Phi_i\rangle-\langle\Psi_f^-|V_i-V_i G_i^+ V_i|\Psi_i^+\rangle. \tag{12b}$$

These are the desired expressions of the stationary Schwinger variational transition matrix elements for rearrangement collisions from the initial bound state i in channel α to the final bound state f in channel β which are next obtained in convenient forms for evaluation using discrete basis sets. It is relevant to note here that these transition matrix elements reduce to those for the direct collisions if $V_f=V_i$ and $G_f^+=G_i^+$.

A. Single-channel formulation of rearrangement collisions

We now make a single-channel expansion of the wave functions Ψ_i^+ and Ψ_f^- in discrete basis sets:

$$\Psi_i^+=\sum_m a_m u_m, \quad \Psi_f^-=\sum_n b_n v_n, \tag{13}$$

where the linear expansion coefficients $a_m=(a_m^{(r)},a_m^{(i)})\equiv(a_m^{(1)},a_m^{(2)})$ and $b_n=(b_n^{(r)},b_n^{(i)})\equiv(b_n^{(1)},b_n^{(2)})$, are to be determined for choices of the channel wave functions u_m and v_n, and we analyze the post form of the Schwinger transition matrix element. It is now useful to define the three-body amplitude

$$[A_{fi}(\beta\vec{k}_f,\alpha\vec{k}_i)]=(-\mu_f/2\pi)[T_{fi}(\beta\vec{k}_f,\alpha\vec{k}_i)], \tag{14}$$

the two-body amplitudes

$$A_{fm}^{(fp)}(\beta\vec{k}_f,\alpha\vec{k}_i)=(-\mu_f/2\pi)\langle\Phi_f|V_f|u_m\rangle=(A_{fm}^{(f1)},A_{fm}^{(f2)}), \tag{15}$$

$$A_{ni}^{(qi)}(\beta\vec{k}_f,\alpha\vec{k}_i)=(-\mu_f/2\pi)\langle v_n|V_f+V_f G_f^+ V_d|\Phi_i\rangle=(A_{ni}^{(1i)},A_{ni}^{(2i)}), \quad V_d=V_i-V_f, \tag{16}$$

and the double scattering amplitude

$$D_{nm}(\beta\vec{k}_f,\alpha\vec{k}_i)=(-\mu_f/2\pi)\langle v_n|V_f-V_f G_f^+ V_f|u_m\rangle=(D_{nm}^{(r)},D_{nm}^{(i)}), \tag{17}$$

with the three-body reduced mass in the final channel $\mu_f=(m_1+m_2)m_3/(m_1+m_2+m_3)$. The post form of the variational amplitude thus takes the form

$$[A_{fi}(\beta\vec{k}_f,\alpha\vec{k}_i)]_{\rm post}=\sum_m A_{fm}a_m+\sum_n b_n^* A_{ni}-\sum_m\sum_n b_n^* D_{nm}a_m . \tag{18}$$

The linear variational parameters $a_m^{(p)}$ and $b_n^{(q)}$ are determined by exploiting the stationary property of $[A_{fi}]_{\rm post}$:

$$\frac{\partial}{\partial a_m^{(p)}}[A_{fi}]_{\rm post}=0=\frac{\partial}{\partial b_n^{(q)}}[A_{fi}]_{\rm post}, \quad m,n=1,2,\ldots,N, \quad p,q=1,2. \tag{19}$$

On differentiating with respect to $a_m^{(p)}$, one obtains

$$0=A_{fm}-\sum_n b_n^* D_{nm}, \quad m=1,2,\ldots,N$$

which yields

$$\sum_n [b_n^{(r)}D_{nm}^{(r)}-b_n^{(i)}D_{nm}^{(i)}]=A_{fm}^{(f1)}, \quad \sum_n [b_n^{(r)}D_{nm}^{(i)}+b_n^{(i)}D_{nm}^{(r)}]=A_{fm}^{(f2)}, \quad m=1,2,\ldots,N. \tag{20}$$

Defining multiplication of complex quantities in terms of array (matrix) multiplication, such as

$$(x+iy)(a+ib)=\begin{pmatrix} x & -y \\ y & x \end{pmatrix}\begin{pmatrix} a \\ b \end{pmatrix}=\begin{pmatrix} a & -b \\ b & a \end{pmatrix}\begin{pmatrix} x \\ y \end{pmatrix}, \quad (21)$$

the above set of linear equations may be written in matrix notation as

$$(\underline{b}_N^{(r)\dagger}\underline{b}_N^{(i)\dagger})\begin{pmatrix} \underline{D}_{N\times N}^{(r)} & -\underline{D}_{N\times N}^{(i)} \\ \underline{D}_{N\times N}^{(i)} & \underline{D}_{N\times N}^{(r)} \end{pmatrix}=(\underline{A}_{fN}^{(f1)} \quad \underline{A}_{fN}^{(f2)}) \quad (22)$$

where the vector coefficients are given by

$$\underline{b}_N^{(r)\dagger}=(b_1^{(r)}b_2^{(r)}\cdots b_N^{(r)}), \quad \underline{b}_N^{(i)\dagger}=(b_1^{(i)}b_2^{(i)}\cdots b_N^{(i)}),$$

$$\underline{b}_N=\begin{pmatrix} \underline{b}_N^{(r)} \\ \underline{b}_N^{(i)} \end{pmatrix}\equiv\begin{pmatrix} \underline{b}_N^{(1)} \\ \underline{b}_N^{(2)} \end{pmatrix}, \quad (23)$$

the submatrices are obtained as

$$\underline{D}_{N\times N}^{(r)}=\begin{pmatrix} D_{11}^{(r)} & D_{12}^{(r)} & \cdots & D_{1N}^{(r)} \\ D_{21}^{(r)} & D_{22}^{(r)} & \cdots & D_{2N}^{(r)} \\ \cdots & \cdots & \cdots & \cdots \\ D_{N1}^{(r)} & D_{N2}^{(r)} & \cdots & D_{NN}^{(r)} \end{pmatrix}\equiv\underline{D}_{N\times N}^{(11)}, \quad (24a)$$

$$\underline{D}_{N\times N}^{(i)}=\begin{pmatrix} D_{11}^{(i)} & D_{12}^{(i)} & \cdots & D_{1N}^{(i)} \\ D_{21}^{(i)} & D_{22}^{(i)} & \cdots & D_{2N}^{(i)} \\ \cdots & \cdots & \cdots & \cdots \\ D_{N1}^{(i)} & D_{N2}^{(i)} & \cdots & D_{NN}^{(i)} \end{pmatrix}\equiv-\underline{D}_{N\times N}^{(12)}, \quad (24b)$$

$$\underline{D}_{N\times N}^{(21)}=-\underline{D}_{N\times N}^{(12)}, \underline{D}_{N\times N}^{(22)}=\underline{D}_{N\times N}^{(11)}, \underline{D}_{2N\times 2N}=\begin{pmatrix} \underline{D}_{N\times N}^{(11)} & \underline{D}_{N\times N}^{(12)} \\ \underline{D}_{N\times N}^{(21)} & \underline{D}_{N\times N}^{(22)} \end{pmatrix}, \quad (25)$$

and the nonhomogeneous column vectors are given as

$$\underline{A}_{fN}^{(f1)}=\begin{pmatrix} A_{f1}^{(f1)} \\ A_{f2}^{(f1)} \\ \vdots \\ A_{fN}^{(f1)} \end{pmatrix}, \quad A_{fN}^{(f2)}=\begin{pmatrix} A_{f1}^{(f2)} \\ A_{f2}^{(f2)} \\ \vdots \\ A_{fN}^{(f2)} \end{pmatrix}, \quad (26)$$

so that the solution for the coefficients $\underline{b}_N^{\dagger}$ is obtained as

$$\underline{b}_N^{\dagger}=(\underline{A}_{fN}^{(f1)}\,\underline{A}_{fN}^{(f2)})\underline{D}_{2N\times 2N}^{(-1)}, \quad (27)$$

which on expansion reads as

$$\underline{b}_N^{(q)}=\sum_{p=1}^{2}\underline{A}_{fN}^{(fp)}\underline{D}_{2N\times 2N}^{(pq)^{-1}}, \quad q=1,2. \quad (28)$$

Thus the coefficients are given by

$$b_n^{(q)}=\sum_{m=1}^{N}\sum_{p=1}^{2}A_{fm}^{(fp)}D_{mn}^{(fp)^{-1}}, \quad q=1,2; \quad n=1,2,\ldots,N, \quad (29)$$

where $D_{mn}^{(pq)^{-1}}$ are the elements of the inverse matrix $\underline{D}_{2N\times 2N}^{-1}$.

Similarly, $(\partial/\partial b_n^{(q)})\,[A_{fi}]_{\text{post}}=0$ yields

$$0=A_{ni}-\sum_m D_{nm}a_m, \quad n=1,2,\ldots,N. \quad (30)$$

which gives rise to

$$\underline{a}_N^{(p)}=\sum_{q=1}^{2}\underline{D}_{2N\times 2N}^{(pq)^{-1}}\underline{A}_{Ni}^{(qi)}, \quad a_m^{(p)}=\sum_{n=1}^{N}\sum_{q=1}^{2}D_{mn}^{(pq)^{-1}}A_{ni}^{(qi)}, \quad p=1,2, \quad m=1,2,\ldots,N. \quad (31)$$

On substitution of these values of $a_m^{(p)}$ and $b_n^{(q)}$ in the expression for $[A_{fi}]_{\text{post}}$, one finally obtains the Schwinger variational amplitude for rearrangement collisions from the bound state i in channel α to the state f in channel β as

$$[A_{fi}(\beta\vec{k}_f,\alpha\vec{k}_i)]_{\text{post}}=\sum_{m,n}\sum_{p,q}A_{fm}^{(fp)}(\beta\vec{k}_f,\alpha\vec{k}_i)D_{mn}^{(pq)^{-1}}A_{ni}^{(qi)}(\beta\vec{k}_f,\alpha\vec{k}_i). \quad (32)$$

In order to evaluate this amplitude, one requires a knowledge of the ''input'' two-body amplitudes $A_{fm}^{(fp)}$ and $A_{ni}^{(qi)}$ and the elements of the double-scattering matrix $\underline{D}_{2N\times 2N}$. These are given in terms of the channel basis functions u_m and v_n. The scattering amplitude is then a function of the scattering angles associated with the vector $\vec{k}_f$, while the incident direction of $\vec{k}_i$ is generally associated with the z axis. Evaluation of the double-scattering terms, however, involve three-dimensional integrals of the intermediate off-shell energies of the final-state Green's function:

$$G_f^{+}=\frac{1}{(2\pi)^3}\sum_{\gamma}\int d\vec{k}^{s}\,\frac{|\Phi_\gamma''\rangle\langle\Phi_\gamma''|}{E-E_\gamma''+i\epsilon}. \quad (33)$$

In fact the double-scattering amplitude takes the form

$$D_{nm}(\beta\vec{k}_f,\alpha\vec{k}_i)=A_{nm}(\beta\vec{k}_f,\alpha\vec{k}_i)-\frac{1}{(2\pi)^3}\sum_{\gamma}\int d\vec{k}''\,\frac{A_{n\gamma}(\beta\vec{k}_f,\gamma\vec{k}'')A_{\gamma m}(\gamma\vec{k}'',\alpha\vec{k}_i)}{E-E_\gamma''+i\epsilon}\left(-\frac{2\pi}{\mu_\gamma}\right), \quad (34)$$

in which we have used definitions

$$A_{nm}(\beta\vec{k}_f,\alpha\vec{k}_i)=(-\mu_f/2\pi)\langle v_n|V_f|u_m\rangle, \tag{35}$$

$$A_{n\gamma}(\beta\vec{k}_f,\gamma\vec{k}'')=(-\mu_f/2\pi)\langle v_n|V_f|\Phi''_\gamma\rangle, \tag{36}$$

$$A_{\gamma m}(\gamma\vec{k}'',\alpha\vec{k}_i)=(-\mu_\gamma/2\pi)\langle\Phi''_\gamma|V_i|u_m\rangle, \tag{37}$$

where the plane-wave states Φ''_γ belong to the final-channel Hamiltonian H_f with off-shell energies E''_γ $(E\neq E''_\gamma)$.

The double-scattering amplitude can be conveniently reduced to a form involving only a single-dimensional principal-value integral after performing the angular integrations, if the partial-wave analysis is allowed to be performed by splitting the pole term $1/(E-E''_\gamma+i\epsilon)$ into a δ-function part and a principal-value part as follows:

$$\frac{1}{E-E''_\gamma\pm i\epsilon}=\mp i\pi\delta(E-E''_\gamma)+P\,\frac{1}{E-E''_\gamma}. \tag{38}$$

An analysis is thus given above for the evaluation of the post form of the Schwinger variational amplitude for rearrangement collisions using discrete basis sets. One can proceed similarly for the study of the prior amplitude $[A_{fi}(\beta\vec{k}_f,\alpha\vec{k}_i)]$ involving the Green's operator G_i^+. In this case the intermediate plane-wave states belong to the incident channel Hamiltonian H_i.

B. Relation to the second Born approximation

The reduction of the Schwinger variational amplitude to the second Born amplitude and its relation to the Padé approximation and other variational methods is an old subject of substantial importance and interest, and has drawn attention of the experts in the field [26–28]. In his derivation of the Schwinger principle for rearrangement collisions, Joachain [9,10] also gave the limiting forms of the amplitudes in post and prior forms under certain restrictions. If in the finite discrete basis set for $m,n=1,2,\ldots,N$, we keep only one term for $N=1$ such that $u_m=A\Phi_i$, $v_n=B\Phi_f$ of plane-wave states as in the Born approximations, and vary the amplitude $[A_{fi}(\beta\vec{k}_f,\alpha\vec{k}_i)]$ with respect to the parameters A and B, we obtain, on neglection of higher-order terms, the following approximate expressions:

$$g^{(\mathrm{post})}_{\mathrm{SBA}}(\beta\vec{k}_f,\alpha\vec{k}_i)=g^{(\mathrm{post})}_{I}(\beta\vec{k}_f,\alpha\vec{k}_i)+g^{(\mathrm{post})}_{II}(\beta\vec{k}_f,\alpha\vec{k}_i), \tag{39}$$

$$g^{(\mathrm{prior})}_{\mathrm{SBA}}(\beta\vec{k}_f,\alpha\vec{k}_i)=g^{(\mathrm{prior})}_{I}(\beta\vec{k}_f,\alpha\vec{k}_i)+g^{(\mathrm{prior})}_{II}(\beta\vec{k}_f,\alpha\vec{k}_i), \tag{40}$$

where

$$g^{(\mathrm{post})}_{I}(\beta\vec{k}_f,\alpha\vec{k}_i)=-(\mu_f/2\pi)T^{(\mathrm{post})}_{I}(\beta\vec{k}_f,\alpha\vec{k}_i), \tag{41}$$

$$g^{(\mathrm{post})}_{II}(\beta\vec{k}_f,\alpha\vec{k}_i)=-(\mu_f/2\pi)T^{(\mathrm{post})}_{II}(\beta\vec{k}_f,\alpha\vec{k}_i), \tag{42}$$

$$g^{(\mathrm{prior})}_{I}(\beta\vec{k}_f,\alpha\vec{k}_i)=-(\mu_f/2\pi)T^{(\mathrm{prior})}_{I}(\beta\vec{k}_f,\alpha\vec{k}_i), \tag{43}$$

$$g^{(\mathrm{prior})}_{II}(\beta\vec{k}_f,\alpha\vec{k}_i)=-(\mu_f/2\pi)T^{(\mathrm{prior})}_{II}(\beta\vec{k}_f,\alpha\vec{k}_i). \tag{44}$$

This essential feature of reducing the Schwinger amplitude to the second-order Born approximation (SBA) is of importance to the study of rearrangement collisions, as has been emphasized earlier and has been highlighted as an attractive characteristic of this variational principle [9,10].

C. Multichannel formulation of rearrangement collisions

It is shown how the formulation can be utilized for a study of rearrangement collisions with the consideration of multichannel expansions of the full wave functions Ψ_i^+ and Ψ_f^- instead of single-channel expansions. While doing this, it is to be borne in mind that the Schwinger amplitude for rearrangement collisions would reduce to the direct collisions, if $V_f=V_i$ and $G_f^+=G_i^+$ for the incident as well as final channels. Indeed, we make use of the expansions

$$\Psi_i^+=\sum_{m=1}^{N}\sum_{a=1}^{2}a_m^{(a)}u_m^{(a)}, \tag{45}$$

$$\Psi_f^-=\sum_{n=1}^{N}\sum_{b=1}^{2}b_n^{(b)}v_n^{(b)}, \tag{46}$$

where $a_m^{(a)}=(a_m^{(ar)},a_m^{(ai)})$ and $b_n^{(b)}=(b_n^{(br)},b_n^{(bi)})$, $a,b=1$ and 2, are the linear variational constants, and $(u_m^{(1)},v_n^{(1)})$ denote wave functions for the incident channel, while $(u_m^{(2)},v_n^{(2)})$ denote those for the final channel.

Defining the two-body amplitudes

$$A^{(fa)}_{fm}(\beta\vec{k}_f,\alpha\vec{k}_i)=-(\mu_f/2\pi)\langle\Phi_f|V_f|u_m^{(a)}\rangle, \tag{47}$$

$$A^{(bi)}_{ni}(\beta\vec{k}_f,\alpha\vec{k}_i)=-(\mu_f/2\pi)\langle v_n^{(b)}|V_f+V_fG_f^+V_d|\Phi_i\rangle \qquad (V_d=V_i-V_f) \tag{48}$$

and the double-scattering amplitude

$$D^{(ba)}_{nm}(\beta\vec{k}_f,\alpha\vec{k}_i)=-(\mu_f/2\pi)\langle v_n^{(b)}|V_f-V_fG_f^+V_f|u_m^{(a)}\rangle, \tag{49}$$

we obtain the post form of the Schwinger amplitudes as

$$[A_{fi}(\beta\vec{k}_f,\alpha\vec{k}_i)]_{\mathrm{post}}=\sum_m\sum_a A^{(fa)}_{fm}(\beta\vec{k}_f,\alpha\vec{k}_i)a_m^{(a)} +\sum_n\sum_b b_n^{(b)*}A^{(bi)}_{ni}(\beta\vec{k}_f,\alpha\vec{k}_i) -\sum_{m,n}\sum_{a,b}b_n^{(b)*}D^{(ba)}_{nm}(\beta\vec{k}_f,\alpha\vec{k}_i)a_m^{(a)} \tag{50}$$

with

$$D^{(ba)}_{nm}=(P^{(ba)}_{nm},Q^{(ba)}_{nm}), \quad A^{(sr)}_{pq}=(R^{(sr)}_{pq},S^{(sr)}_{pq}). \tag{51}$$

On optimization of $[A_{fi}]_{\mathrm{post}}$ with respect to variational parameters $a_m^{(a)}$ and $b_n^{(b)}$, $m,n=1,2,\ldots,N$, $a,b=1,2$, so that

$$\frac{\partial}{\partial a_m^{(a)}}[A_{fi}]_{\text{post}}=0=\frac{\partial}{\partial b_n^{(b)}}[A_{fi}]_{\text{post}}, \tag{52}$$

one obtains

$$(\underline{b}_N^{(br)},\underline{b}_N^{(bi)})=(\underline{R}_{fN}^{(fa)},-\underline{S}_{fN}^{(fa)})\underline{D}_{4N\times 4N}^{(ab)^{-1}}, \tag{53}$$

where $\underline{D}_{4N\times 4N}^{(ab)^{-1}}$ denotes the inverse matrix corresponding to $\underline{D}_{4N\times 4N}^{(ab)}$ consisting of block matrices $\underline{P}_{N\times N}^{(ab)}$, $Q_{N\times N}^{(ab)}$, so that

$$\underline{D}_{4N\times 4N}^{(ab)}=\begin{pmatrix}\underline{P}_{2N\times 2N}^{(ab)} & -Q_{2N\times 2N}^{(ab)}\\ Q_{2N\times 2N}^{(ab)} & \underline{P}_{2N\times 2N}^{(ab)}\end{pmatrix}, \tag{54}$$

$$\underline{P}_{2N\times 2N}^{(ab)}=\begin{pmatrix}\underline{P}_{N\times N}^{(11)} & \underline{P}_{N\times N}^{(12)}\\ \underline{P}_{N\times N}^{(21)} & \underline{P}_{N\times N}^{(22)}\end{pmatrix},\quad Q_{2N\times 2N}^{(ab)}=\begin{pmatrix}Q_{N\times N}^{(11)} & Q_{N\times N}^{(12)}\\ Q_{N\times N}^{(21)} & Q_{N\times N}^{(22)}\end{pmatrix},$$

and

$$(\underline{R}_{fN}^{(fa)},-\underline{S}_{fN}^{(fa)})=(R_{f1}^{(f1)},R_{f2}^{(f1)},\ldots,R_{fN}^{(f1)},R_{f1}^{(f2)},R_{f2}^{(f2)},\ldots,R_{fN}^{(f2)},-S_{f1}^{(f1)},-S_{f2}^{(f1)},\ldots,-S_{fN}^{(f1)},-S_{f1}^{(f2)},-S_{f2}^{(f2)},\ldots,-S_{fN}^{(f2)}) \tag{55}$$

Similarly, the coefficients $a_m^{(a)}$ are given by

$$\begin{pmatrix}\underline{a}_N^{(ar)}\\ \underline{a}_N^{(ai)}\end{pmatrix}=\underline{D}_{4N\times 4N}^{(ab)^{-1}}\begin{pmatrix}\underline{R}_{Ni}^{(bi)}\\ \underline{S}_{Ni}^{(bi)}\end{pmatrix}. \tag{56}$$

Finally thus the multichannel Schwinger amplitude for rearrangement collisions is obtained as

$$\begin{pmatrix}[A_{fi}^{(R)}(\beta\vec{k}_f,\alpha\vec{k}_i)]_{\text{post}}\\ [A_{fi}^{(I)}(\beta\vec{k}_f,\alpha\vec{k}_i)]_{\text{post}}\end{pmatrix}=\sum_{m,n}\sum_{a,b}(\underline{R}_{fN}^{(fa)},-\underline{S}_{fN}^{(fa)})\underline{D}_{4N\times 4N}^{(ab)^{-1}}\begin{pmatrix}\underline{R}_{Ni}^{(bi)}\\ \underline{S}_{Ni}^{(bi)}\end{pmatrix}. \tag{57}$$

In this form, it is convenient to evaluate accurate variational amplitudes if the input two-body amplitudes are defined with a proper choice of the basis functions $u_m^{(a)}$ and $v_n^{(b)}$, $a,b=1,2$, which must contain, as a matter of fact, nonlinear variational parameters and sufficiently flexible correlation terms. Since this formulation has been defined for two channels, the amplitudes $[A_{ii}(\alpha\vec{k}_i',\alpha\vec{k}_i)]_{\text{post}}$, $[A_{fi}(\beta\vec{k}_f,\alpha\vec{k}_i)]_{\text{post}}$, and $[A_{ff}(\beta\vec{k}_f',\beta\vec{k}_f)]_{\text{post}}$ would describe, respectively, elastic scattering in the direct channel α, rearrangement collisions from the state i in channel α to the state f in channel β, and, finally, elastic scattering in the rearrangement channel β. The two-body amplitudes are to be defined accordingly as required for the nature of scattering to be considered in a calculation.

A similar analysis may as well be done for the prior form of the Schwinger amplitude $[A_{fi}(\beta\vec{k}_f,\alpha\vec{k}_i)]_{\text{prior}}$. It is, however, not known how the results would be predicted by these two forms of the Schwinger amplitude.

III. APPLICATION TO POSITRON-HYDROGEN COLLISIONS

We use the prior form of the Schwinger transition matrix [Eq. (12b)] for Ps formation in the f state in channel β in positron scattering from atomic hydrogen in state i in channel α. If $\vec{r}_1$ and $\vec{r}_2$ denote the position vectors of the incident positron and atomic electron, respectively, with respect to the massive proton at rest at the center of the coordinate system, then $V_i=1/r_1-1/r_{12}$, $V_f=1/r_1-1/r_2$ (a.u.). In the Schrödinger representation, the plane-wave states are obtained as

$$\Phi_i(\vec{r}_1,\vec{r}_2)=\langle\vec{r}_1,\vec{r}_2|\Phi_i\rangle=\exp(i\vec{k}_i\cdot\vec{r}_1)\,\phi_i(\vec{r}_2), \tag{58a}$$

$$\Phi_f(\vec{r}_{12},\vec{s}_{12})=\langle\vec{r}_{12},\vec{s}_{12}|\Phi_f\rangle=\exp(i\vec{k}_f\cdot\vec{s}_{12})\,\eta_f(\vec{r}_{12}), \tag{58b}$$

where the relative coordinate, $\vec{r}_{12}=\vec{r}_1-\vec{r}_2$ and the center-of-mass coordinate $\vec{s}_{12}=1/2(\vec{r}_1+\vec{r}_2)$; $\phi_i(\vec{r}_2)$ and $\eta_f(\vec{r}_{12})$ denote the bound states in the incident and rearrangement channels respectively, with $\hbar\vec{k}_i$ and $\hbar\vec{k}_f$ the momenta of the incident positron and the moving Ps. Energy conservation requires that $E_i=E_f=E$, the total energy of the system, where $E_i=\hbar^2k_i^2/2\mu_i+\epsilon_i$ and $E_f=\hbar^2k_f^2/2\mu_i+\epsilon_f$, (ϵ_i,ϵ_f) and (μ_i,μ_f) denoting, respectively, the eigenenergies and three-body reduced masses in (incident, final) channels. In this representation, the Green's function is obtained as

$$G_i^+(\vec{r}_1,\vec{r}_2;\vec{r}_1',\vec{r}_2')=\frac{1}{(2\pi)^3}\sum_\gamma\int d\vec{k}''\,\frac{\langle\vec{r}_1,\vec{r}_2|\Phi_\gamma''\rangle\langle\Phi_\gamma''|\vec{r}_1',\vec{r}_2'\rangle}{E-E_\gamma''+i\epsilon}. \tag{59}$$

in which the intermediate plane-wave states $|\Phi_\gamma''\rangle$ belong to the incident channel Hamiltonian H_i. We now expand the full wave functions Ψ_i^+ and Ψ_f^- in discrete basis sets of single channel functions:

$$\Psi_i^+=\sum_{m=1}^N a_m u_m,\quad \Psi_f^-=\sum_{n=1}^N b_n v_n. \tag{60}$$

where $a_m=(a_m^{(r)},a_m^{(i)})\equiv(a_m^{(1)},a_m^{(2)})$ and $b_n=(b_n^{(r)},b_n^{(i)})\equiv(b_n^{(1)},b_n^{(2)})$ are linear variational constants. It is now required to define the ''prior'' form of the three-body amplitude from Eq. (12b),

$$[A_{fi}(\beta\vec{k}_f,\alpha\vec{k}_i)]_{\rm prior}=(-\mu_f/2\pi)[T_{fi}(\beta\vec{k}_f,\alpha\vec{k}_i)]_{\rm prior}, \tag{61}$$

the two-body amplitudes

$$A_{fm}(\beta\vec{k}_f,\alpha\vec{k}_i)=(-\mu_f/2\pi)\langle\Phi_f|V_i+V_d^+G_i^+V_i|u_m\rangle \quad (V_d^+=V_f-V_i), \tag{62}$$

$$A_{ni}(\beta\vec{k}_f,\alpha\vec{k}_i)=(-\mu_f/2\pi)\langle v_n|V_i|\Phi_i\rangle, \tag{63}$$

$$A_{nm}(\beta\vec{k}_f,\alpha\vec{k}_i)=(-\mu_f/2\pi)\langle v_n|V_i|u_m\rangle, \tag{64}$$

and the double-scattering amplitude

$$D_{nm}(\beta\vec{k}_f,\alpha\vec{k}_i)=A_{nm}(\beta\vec{k}_f,\alpha\vec{k}_i)-\frac{1}{(2\pi)^3}\sum_\gamma\left(-\frac{2\pi}{\mu_\gamma}\right)\int d\vec{k}''\,\frac{A_{n\gamma}(\beta\vec{k}_f,\gamma\vec{k}'')A_{\gamma m}(\gamma\vec{k}'',\alpha\vec{k}_i)}{E-E''_\gamma+i\epsilon} \tag{65}$$

where $A_{n\gamma}(\beta\vec{k}_f,\gamma\vec{k}'')$ and $A_{\gamma m}(\gamma\vec{k}'',\alpha\vec{k}_i)$ are defined for the intermediate plane-wave states $|\Phi''_\gamma\rangle$.

Let the partial-wave expansion be defined by

$$[A_{fi}(\beta\vec{k}_f,\alpha\vec{k}_i)]_{\rm prior}=\frac{4\pi}{\sqrt{k_fk_i}}\sum_{l,m}[A_{fi}^{(L)}(\beta k_f,\alpha k_i)]_{\rm prior}Y_{lm}(\hat{k}_f)Y_{lm}^*(\hat{k}_i), \tag{66}$$

and similarly for the two-body input amplitudes. On multiplication by $Y_{L0}^*(\hat{k}_f)$ and integration over $\hat{k}_f$, one obtains with the help of orthogonal properties of the spherical harmonics:

$$\int Y_{L0}^*(\hat{k}_f)[A_{fi}(\beta\vec{k}_f,\alpha\vec{k}_i)]d\hat{k}_f=\frac{4\pi}{\sqrt{k_fk_i}}[A_{fi}(\beta k_f,\alpha k_i)]Y_{L0}(\hat{k}_i). \tag{67}$$

If we choose the direction of incidence along the z axis, $\vec{k}_i=(k_i,0,0)$, it would give $\hat{k}_i,\hat{k}_f=\cos\theta_f$, $Y_{L0}(\hat{k}_f)=\sqrt{(2L+1)/4\pi}P_L(\cos\theta_f)$, $d\hat{k}_f=\sin\theta_f d\theta_f d\phi_f$, and thus on integration over ϕ_f, we finally obtain the partial-wave scattering amplitude as

$$[A_{fi}^{(L)}(\beta k_f,\alpha k_i)]_{\rm prior}=\sqrt{k_ik_f}/2\int_{-1}^{+1}[A_{fi}(\beta\vec{k}_f,\alpha\vec{k}_i)]_{\rm prior}P_L(\cos\theta_f)d(\cos\theta_f). \tag{68}$$

In order to perform the partial-wave analysis of the amplitudes involving the pole term $1/(E-E''_\gamma\pm i\epsilon)$, we split it into a δ-function part and a principle-value part:

$$1/(E-E''_\gamma\pm i\epsilon)=\mp i\pi\delta(E-E''_\gamma)+P\,\frac{1}{E-E''_\gamma}. \tag{69}$$

Similarly, these are obtained as

$$A_{fm}^{(L)}(\beta k_f,\alpha k_i)=G_{fm}^{(L)}(\beta k_f,\alpha k_i)+i\sum_\gamma H_{f\gamma}^{(L)}(\beta k_f,\alpha k_\gamma)F_{\gamma m}^{(L)}(\alpha k_\gamma,\alpha k_i)$$
$$-\frac{2}{\pi\hbar^2}\sum_\gamma P\int_0^\infty\frac{k''dk''}{k_\gamma^2-k''^2}H_{f\gamma}^{(L)}(\beta k_f,\alpha k'')F_{\gamma m}^{(L)}(\alpha k'',\alpha k_i)=(A_{fm}^{(r)},A_{fm}^{(i)}), \tag{70}$$

$$D_{nm}^{(L)}(\beta k_f,\alpha k_i)=A_{nm}^{(L)}(\beta k_f,\alpha k_i)-i\sum_\gamma A_{n\gamma}^{(L)}(\beta k_f,\alpha k_\gamma)A_{\gamma m}^{(L)}(\alpha k_\gamma,\alpha k_i)$$
$$+\frac{2}{\pi\hbar^2}\sum_\gamma P\int_0^\infty\frac{k''dk''}{k_\gamma^2-k''^2}A_{n\gamma}^{(L)}(\beta k_f,\alpha k'')A_{\gamma m}^{(L)}(\alpha k'',\alpha k_i)=(D_{nm}^{(r)},D_{nm}^{(i)}), \tag{71}$$

TABLE I. The present partial-wave contributions to the ground-state positronium formation cross section (πa_0^2) in e^+-hydrogen collisions in the energy range 6.8–30.0 eV. The notation $x[-y]$ stands for $x \times 10^{-y}$. $^\dagger\sigma_t$ includes all significant partial-wave contributions.

E (eV) / L	6.855 76	7.65	8.704	9.826	10.2	11.0	12.0
0	0.0041	0.0043	0.0049	0.0058	0.0062	0.0069	0.0075
	0.0041[a]	0.0044[a]	0.0049[a]	0.0058[a]			
	0.404[−2][b]	0.426[−2][b]	0.480[−2][b]	0.550[−2][b]			
1	0.0270	0.3639	0.483	0.5614	0.6032	0.6568	0.6777
	0.027[a]	0.365[a]	0.482[a]	0.561[a]			
	0.267[−1][b]	0.366[b]	0.483[b]	0.564[b]			
2	0.00062	0.3350	0.8119	1.0569	1.1021	1.2421	1.2816
	0.00062[a]	0.335[a]	0.812[a]	1.057[a]			
	0.682[−3][b]	0.321[b]	0.860[b]	1.158[b]			
3	0.5037[−5]	0.3536[−1]	0.2717	0.5553	0.6089	0.6240	0.6416
	0.445[−5][b]	0.357[−1][b]	0.271[b]	0.595[b]			
4	0.3875[−6]	0.1092[−1]	0.1113	0.2917	0.3320	0.3485	0.3602
5	0.1559[−8]	0.1182[−2]	0.2537[−1]	0.1115	0.1503	0.1711	0.1878
6		0.5294[−4]	0.2543[−2]	0.0181	0.0268	0.0399	0.6248[−1]
7		0.2505[−5]	0.2285[−3]	0.2651[−2]	0.4325[−2]	0.7583[−2]	0.1550[−1]
8		0.8375[−7]	0.1676[−4]	0.3502[−3]	0.6461[−3]	0.1335[−2]	0.4080[−2]
9		0.3892[−8]	0.1636[−5]	0.4580[−4]	0.9080[−4]	0.2204[−3]	0.7960[−3]
10			0.1165[−6]	0.4660[−5]	0.1183[−4]	0.3436[−4]	0.1472[−3]
11			0.9106[−8]	0.5418[−6]	0.1578[−5]	0.2056[−4]	0.2663[−4]
12			0.4579[−9]	0.6115[−7]	0.1615[−6]	0.6248[−6]	0.3503[−5]
13					0.1918[−7]	0.8183[−7]	0.5837[−6]
14					0.2248[−8]	0.1010[−7]	0.9471[−7]
15						0.1362[−8]	0.1509[−7]
$\sigma_t^\dagger$	0.0317	0.7507	1.7110	2.6037	2.8346	3.0985	3.2394
$\sigma_t^{\dagger}$[b]	0.0314[−1][b]	0.730[b]	1.663[b]	2.492[b]			

E (eV) / L	13.6	15.0	18.5	20.0	26.0	30.0
0	0.0084	0.0089	0.0053	0.0045	0.0142[−1]	0.0677[−2]
1	0.6528	0.6268	0.4188	0.3151	0.1252	0.0986
2	1.3065	1.1501	0.8436	0.7715	0.5733	0.3263
3	0.6624	0.6826	0.7291	0.7172	0.5207	0.4376
4	0.3848	0.4089	0.4444	0.4204	0.2843	0.2610
5	0.2088	0.2229	0.2559	0.2262	0.1734	0.1543
6	0.1204	0.1327	0.1126	0.1072	0.8502[−1]	0.6565[−1]
7	0.4154[−1]	0.6319[−1]	0.5667[−1]	0.5036[−1]	0.3972[−1]	0.3344[−1]
8	0.1043[−1]	0.1821[−1]	0.2005[−1]	0.2257[−1]	0.1717[−1]	0.1573[−1]
9	0.2467[−2]	0.4840[−2]	0.5618[−2]	0.5941[−2]	0.4297[−2]	0.2735[−2]
10	0.5550[−3]	0.1237[−2]	0.1574[−2]	0.1788[−2]	0.1582[−2]	0.1102[−2]
11	0.1209[−3]	0.3057[−3]	0.4172[−3]	0.4398[−3]	0.3571[−3]	0.2276[−3]
12	0.2681[−4]	0.3067[−4]	0.4079[−4]	0.4389[−4]	0.5811[−4]	0.4028[−4]
13	0.3210[−5]	0.4037[−5]	0.1111[−4]	0.1273[−4]	0.1972[−4]	0.1176[−4]
14	0.3241[−6]	0.6231[−6]	0.2941[−5]	0.3569[−5]	0.6539[−5]	0.3948[−5]
15	0.6106[−7]	0.1364[−6]	0.7662[−6]	0.9871[−6]	0.2147[−5]	0.1458[−5]
σ_t	3.3992	3.3207	2.8941	2.6433	1.8266	1.3974

[a]Humberston (1982, 1984), and Brown and Humberston (1985).
[b]Gien (1997).

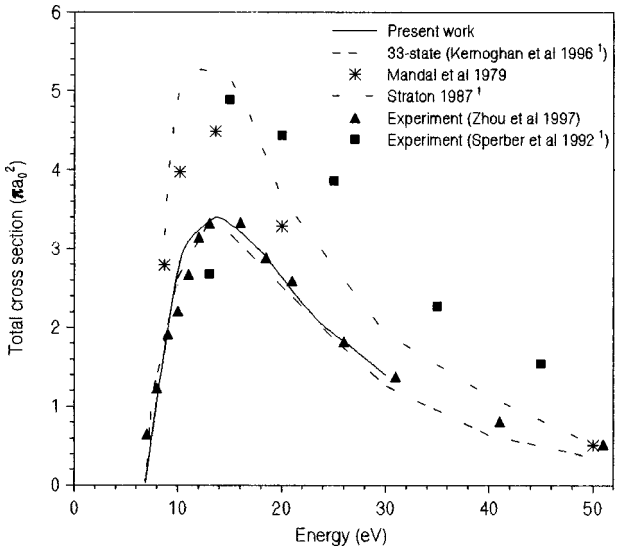

FIG. 1. Total cross sections (πa_0^2) for ground-state positronium formation in positron-hydrogen collisions in the energy range 6.8–52.0 eV.

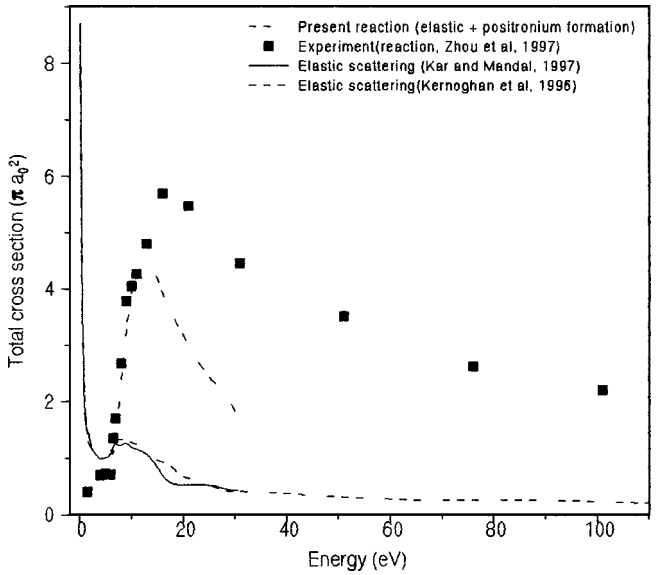

FIG. 2. Total cross sections (πa_0^2) for elastic scattering and net reaction in positron-hydrogen collisions in the incident energy range 0.136–110 eV.

where $G_{fm}^{(L)}$, $H_{f\gamma}^{(L)}$, $F_{\gamma m}^{(L)}$ are the partial-wave amplitudes corresponding to $(-\mu_f/2\pi)\langle\Phi_f|V_i|u_m\rangle$, $(-\mu_f/2\pi)\langle\Phi_f|V_d^+|\Phi_\gamma''\rangle$, and $(-\mu_i/2\pi)\langle\Phi_\gamma''|V_i|u_m\rangle$, respectively. Thus the partial-wave form of the Schwinger amplitude becomes

$$[A_{fi}^{(L)}(\beta k_f,\alpha k_i)]_{\text{prior}}=\sum_{m=1}^{N}A_{fm}^{(L)}(\beta k_f,\alpha k_i)a_m+\sum_{m=1}^{N}b_n^*A_{ni}^{(L)}(\beta k_f,\alpha k_i)-\sum_m\sum_n b_n^*D_{nm}^{(L)}(\beta k_f,\alpha k_i)a_m. \tag{72}$$

The linear variational parameters a_m and b_n are determined by exploiting the stationary property of $[A_{fi}^{(L)}]_{\text{prior}}$:

$$\frac{\partial}{\partial a_m^{(p)}}[A_{fi}^{(L)}]_{\text{prior}}=0=\frac{\partial}{\partial b_n^{(q)}}[A_{fi}^{(L)}]_{\text{prior}},\qquad p,q=1,2,\quad m,n=1,2,\ldots,N. \tag{73}$$

On differentiation with respect to $a_m^{(p)}(p=1$ and 2), one obtains

$$0=A_{fm}^{(L)}-\sum_n b_n^*D_{nm}^{(L)},\quad m=1,2,\ldots,N. \tag{74}$$

Suppressing the superscript for the partial wave L, one realizes that

$$b_n^{(q)}=\sum_{m=1}^{N}\sum_{p=1}^{2}A_{fm}^{(fp)}D_{mn}^{(pq)-1},\qquad q=1,2\quad n=1,2,\ldots,N, \tag{75}$$

which in matrix notation is

$$\underline{b}_N^{(q)}=\sum_{p=1}^{2}\underline{A}_{fN}^{(fp)}\underline{D}_{2N\times 2N}^{(pq)\,-1}, \tag{76}$$

where $D_{nm}^{(pq)^{-1}}$ are the elements of the inverse matrix $D_{2N\times 2N}^{(pq)\,-1}$. Similarly, the other equation yields

$$\underline{a}_N^{(p)}=\sum_{q=1}^{2}\underline{D}_{2N\times 2N}^{(pq)\,-1}\underline{A}_{Ni}^{(pi)},$$

$$a_m^{(p)}=\sum_{n=1}^{N}\sum_{q=1}^{2}\underline{D}_{mn}^{(pq)\,-1}\underline{A}_{ni}^{(qi)},\quad p,=1,2\quad m=1,2,\ldots,N. \tag{77}$$

The linear variational constants are then substituted into the expression for $[A_{fi}^{(L)}]$, to obtain, finally

$$[A_{fi}^{(L)}(\beta k_f,\alpha k_i)]_{\text{prior}}=\sum_{m,n}\sum_{p,q}A_{fm}^{(L)(fp)}(\beta k_f,\alpha k_i)D_{mn}^{(L)(pq)^{-1}}\times A_{ni}^{(L)(qi)}(\beta k_f,\alpha k_i), \tag{78}$$

which has the same structure as in Eq. (32), and is now a function of the scattering energies for each partial wave L. If the partial-wave input amplitudes $A_{fm}^{(L)(fp)}$, $A_{ni}^{(L)(qi)}$, and $A_{nm}^{(L)(pq)^{-1}}$ are supplied for a given choice of the basis functions u_m and v_n, the Schwinger amplitude $[A_{fi}^{(L)}(\beta k_f,\alpha k_i)]_{\text{prior}}$ can be very conveniently evaluated, as we shall see below.

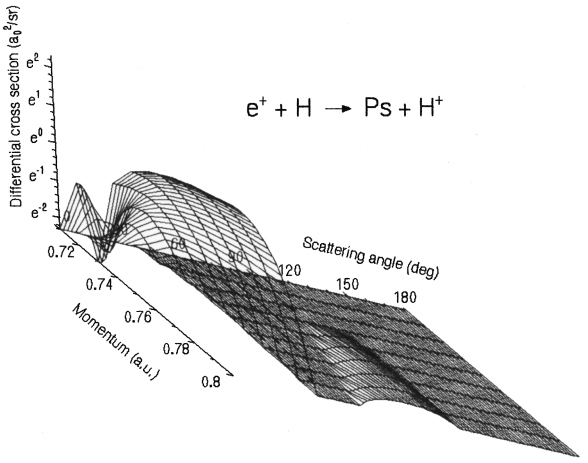

FIG. 3. Surface plot of the differential cross section (a_0^2/sr) for ground-state positronium formation in positron-hydrogen collisions as a function of incident momentum (0.71–0.80 a.u.) and scattering angle (0°–180°).

One of the highlights of our present calculations is the choice of the basis set of the channel functions u_m and v_n. We choose correlated functions with inverse powers of half-odd integers as follows:

$$u_m(\vec{r}_1,\vec{r}_2)=(-1)^{m-1}\xi_m(\vec{r}_1,\vec{r}_2)\Phi_i(\vec{r}_1,\vec{r}_2), \quad (79a)$$

$$v_n(\vec{r}_1,\vec{r}_2)=(-1)^{n-1}\xi_n(\vec{r}_1,\vec{r}_2)\Phi_f(\vec{r}_{12},\vec{s}_{12}), \quad (79b)$$

where the same correlation function $\xi_m(\vec{r}_1,\vec{r}_2)$ is chosen for both the incident $(e^+ + H)$ direct and the final $(Ps + H^+)$ rearrangement channels:

$$\xi_m(\vec{r}_1,\vec{r}_2)=e^{-\alpha_m r_1}/(a+br_{12})^{m_0-1/2}, \quad (80)$$

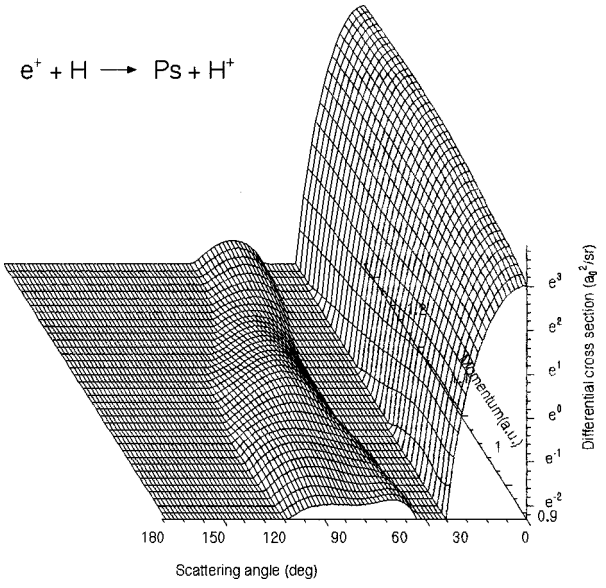

FIG. 4. Surface plot of the differential cross section (a_0^2/sr) for ground-state positronium formation in positron-hydrogen collisions as a function of incident momentum (0.85–1.22 a.u.) and scattering angle (0°–180°).

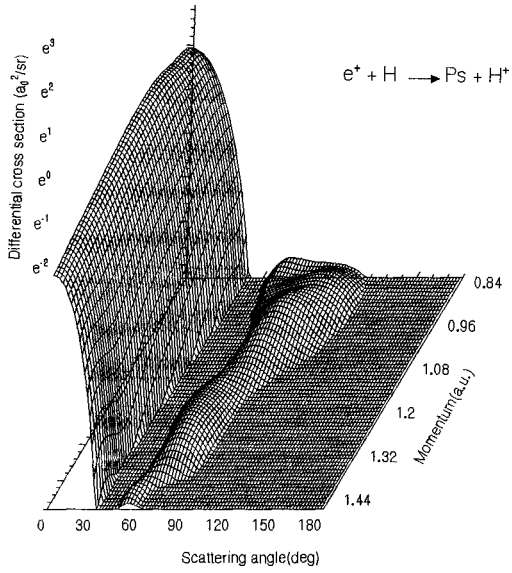

FIG. 5. Surface plot of the differential cross section (a_0^2/sr) for ground-state positronium formation in positron-hydrogen collisions as a function of incident momentum (0.84–1.48 a.u.) and scattering angle (0°–180°).

where $\alpha_{2m}=p$ and $\alpha_{2m-1}=0$, and a, b, and p are nonlinear variational parameters to be optimized with $m_0=1$, for $m=1$ and 2; with $m_0=2$, for $m=3$ and 4; with $m_0=3$, for $m=5$ and 6; with $m_0=4$, for $m=7$ and 8; and so on.

With this choice of the basis set, the input two-body amplitudes are conveniently obtained as a function of the incident energy for each partial wave L. The evaluation of the single-dimensional principal-value integral over $[0,\infty)$ can be performed quite accurately by splitting the range into intervals $[0,2k_\gamma]$ and $[2k_\gamma,\infty)$. Then we use Gauss-Legendre quadrature of an ''even'' number of points for the first interval $[0,2k_\gamma]$, such that the principal-value integral is defined characteristically as $\lim_{\delta\to 0^+}(\int_0^{k_\gamma-\delta}dk''\ldots+\int_{k_\gamma+\delta}^{2k_\gamma}dk''\ldots)$, since the distribution of quadrature points are evenly distributed around the midpoint $k''=k_\gamma$. The evaluation of the integral for the other interval $[2k_\gamma,\infty)$ can be performed in a straightforward manner by using any standard technique. We have, however, used the Gauss-Legendre method with 20 quadrature points for a smooth convergence of the results. In this work, we have included only the ground state of hydrogen with $\gamma=100$ in the summation over intermediate states γ. The effects of the dominant interactions for low-energy collisions are taken care of by the correlated basis functions, which are quite flexible.

IV. RESULTS AND DISCUSSION

The procedure for nonlinear optimization of the variational parameters a, b, and p is as follows. We set $b=1.0$ on the basis of the fact that the normalization of the wave function is not required in defining the Schwinger variational expression for the transition matrix. Next, for a given choice of the variational parameter a, the variational parameter p is varied within a finite range, say, [0.0, 2.5], to search for a stationary range of values of the scattering amplitude $[A_{fi}^{(L)}]_{\text{prior}}$. This process is continued until a suitable combi-

TABLE II. Differential cross section $d\sigma/d\Omega(a_0^2 sr^{-1})$ for positronium formation in atomic hydrogen at incident energy range 6.8–30.0 eV for the scattering angles 0°, 45°, 60°, and 120° along with the critical angle θ_c^0, the ratio $R=4\pi(d\sigma/d\Omega)_{\theta=0}/\sigma$, and the reaction cross section σ_τ. The notation $x[-y]$ stands for $x\times10^{-y}$.

Angle	$d\sigma/d\Omega$						
E (eV)	0°	45°	60°	120°	θ_c^0	R	σ_τ
6.85576	0.2209[−1]	0.6561[−2]	0.1683[−2]	0.1149[−1]	73.40	8.761	1.2878
7.65	0.2616[+1]	0.1361	0.0061[−2]	0.9825[−1]	60.20	43.786	1.9724
8.704	0.9992[+1]	0.4500[−1]	0.6150[−1]	0.9342[−1]	50.02	73.386	2.9802
9.826	2.0372[+1]	0.0579[−2]	1.4407[−1]	0.9144[−1]	44.80	98.322	3.8126
10.2	2.3565[+1]	0.2867[−1]	1.4414[−1]	0.9660[−1]	44.01	104.469	4.0344
11.0	2.6900[+1]	0.1766[−2]	0.1291	0.1084	44.25	109.096	4.2623
12.0	3.0342[+1]	0.0924[−2]	0.1198	0.1139	44.60	117.704	4.3626
13.6	3.7642[+1]	0.1896[−2]	0.8228[−1]	0.9185[−1]	44.00	139.157	4.4154
15.0	4.0725[+1]	0.3232[−2]	0.8271[−1]	0.8981[−1]	43.26	154.114	4.1612
18.5	3.8548[+1]	0.4244[−1]	0.1367	0.4711[−1]	39.20	167.378	3.4389
20.0	3.5836[+1]	0.5215[−1]	0.1613	0.2749[−1]	38.55	170.366	3.1789
26.0	2.5676[+1]	0.6550[−1]	0.1366	0.4560[−2]	36.85	176.642	2.3357
30.0	2.0253[+1]	0.8416[−1]	0.1102	0.3261[−2]	35.20	182.129	1.8279

nation of the values of a and p is discovered up to a satisfactory level of accuracy. It is worthwhile to note that a remarkable stability in the calculations was achieved with only $N=8$ terms in the basis expansion for the energy range considered in the present work (6.8–30.0 eV), for all values of the partial wave $L=0-15$.

A. Total cross sections

The values of the S, P, D, and higher partial-wave cross sections for ground-state Ps formation in hydrogen are shown in Table I, along with available variational results for incident positron energies in the range 6.8–30.0 eV. As is apparent, the present Schwinger variational results are in accord with available Kohn-Hulthĕn and Harris-Nesbet values [13,14]. There is, however, a wide range of calculations available in the literature using a variety of approximation methods, a comprehensive review of which is available in the literature [6,7,11–23,29]. It is of interest to note that the recent results of the 33-state coupled-state calculation of Kernoghan *et al.* [20] and the 28-state close coupling approximation of Mitroy [21] are in satisfactory agreement with our studies.

The total ground-state Ps formation cross sections are displayed in Fig. 1 along with other theoretical predictions [16,18,20] and the observed data of Zhou *et al.* [23] and Sperber *et al.* [22]. The recent measurement of Zhou *et al.* [23] agrees nicely with our predictions over the entire energy range (6.8–30.0 eV) considered in our calculation. The general shape of the cross section is similar in both cases—it rises from the threshold steadily to show a peak value at around 15.0 eV and then falls off with the increase of positron energy. Our values of the total Ps formation cross section are interestingly smaller than those predicted by the Fock-Tani calculation in the energy range below 30 eV. The observed data of Sperber *et al.* [22] are available from around 15.0 eV for the total formation cross section into all states of Ps. These data are reasonably consistent with the observed data of Zhou *et al.* [23], the earlier measurements overestimating the latter. The recent observations of Zhou *et al.* [23] agree with the recent coupled 33-state calculation of Kernoghan *et al.* [20] and the 28-state close-coupling approximation calculation of Mitroy [21] (not included in the figure). As is evident, the agreement between our present Schwinger variational calculation and the 33-state calculation of Kernoghan *et al.* [20] is remarkably close at low energies below 10.2 eV, and quite reasonable beyond this energy. The distorted-wave results of Ref. [16] are not expected to be valid at low-energies. They overestimate the present results and the observed data [23] below 50 eV, beyond which, however, the estimated cross sections [16] are in reasonable agreement with the experiment [23].

The present Schwinger variational results and the measurements of Zhou *et al.* [23] are further compared in Fig. 2 in which we have drawn curves of the total elastic and the total reaction (elastic plus Ps formation) cross sections as given by the Schwinger variational method [7] along with the elastic results of Kernoghan *et al.* [20]. The comparison reveals interesting findings. While the elastic cross section predicted by all the theoretical methods are in complete accord among themselves [7,20,21], the measured values are quite smaller than these predictions below 6.8 eV. The Schwinger reaction cross section is the sum of the total elastic [7] and the present ground-state Ps formation cross sections. The values are in very good agreement with the observed data of Zhou *et al.* [23] in the incident positron energy range 6.8–10.2 eV, the Oré gap, in which only elastic scattering and Ps formation are energetically allowed. Beyond 10.2 eV, the inelastic channels are all open including the ionization from 13.6 eV. Naturally the observed data are of greater magnitude than the present results at energies beyond 10.2 eV.

B. Differential cross sections

One other interesting aspect of the present calculation is the prediction of critical angles in Ps formation as displayed

TABLE III. Differential cross section $d\sigma/d\Omega(a_0^2/sr)$ for positronium formation in hydrogen at incident positron energies 6.855 76, 8.704, 10.2, 13.6, 20.0, 26.0, and 30.0 eV. The notation $a\pm b$ stands for $a\times10^{\pm b}$.

E (eV) Angle (deg)	6.85576	8.704	10.2	13.6	20.0	26.0	30.0
0.0	0.2209−1	0.9992+1	2.3565+1	3.7642+1	3.5836+1	2.5676+1	2.0253+1
5.0	0.2180−1	0.9523+1	2.2060+1	3.4310+1	3.2137+1	2.2958+1	1.8139+1
10.0	0.2096−1	0.8235+1	1.8072+1	2.5967+1	2.3118+1	1.6326+1	1.2905+1
15.0	0.1961−1	0.6443+1	1.2892+1	1.6287+1	1.3241+1	0.9116+1	0.7130+1
20.0	0.1784−1	0.4533+1	0.7922+1	0.8422+1	0.5957+1	0.3925+1	0.2969+1
25.0	0.1575−1	0.2837+1	0.4102+1	0.3545+1	0.2039+1	0.1249+1	0.8712
30.0	0.1346−1	0.1546+1	0.1706+1	0.1174+1	0.4796	0.2501	0.1375
35.0	0.1109−1	0.7035	0.5042	0.2762	0.4824−1	0.1211−1	0.1647−2
40.0	0.8750−2	0.2416	0.6736−1	0.3047−1	0.5672−2	0.1853−1	0.3833−1
45.0	0.6561−2	0.4500−1	0.2867−2	0.1896−2	0.5215−1	0.6550−1	0.8416−1
50.0	0.4609−2	0.0082−2	0.5807−1	0.2356−1	0.1015	0.1003	0.1051
55.0	0.2965−2	0.2224−1	0.1157	0.5169−1	0.1384	0.1224	0.1108
60.0	0.1683−2	0.6150−1	1.4414−1	0.8228−1	0.1613	0.1366	0.1102
65.0	0.0791−2	0.9539−1	0.1490	0.1180	0.1685	0.1411	0.1021
70.0	0.0382−2	0.1180	0.1436	0.1582	0.1603	0.1340	0.8519−1
75.0	0.0210−2	0.1310	0.1379	0.1971	0.1417	0.1194	0.6499−1
80.0	0.0497−2	0.1377	0.1363	0.2263	0.1196	0.1023	0.4570−1
90.0	0.2073−2	0.1422	0.1456	0.2345	0.7896−1	0.6495−1	0.1876−1
100.0	0.4697−2	0.1385	0.1532	0.1886	0.5188−1	0.3267−1	0.7304−2
110.0	0.7971−2	0.1226	0.1368	0.1329	0.3931−1	0.1572−1	0.5876−2
120.0	0.1149−1	0.9342−1	0.9660−1	0.9185−1	0.2749−1	0.4560−2	0.3261−2
140.0	0.1794−1	0.2903−1	0.2820−1	0.4012−1	0.1345−1	0.0251−2	0.0426−2
160.0	0.2219−1	0.2943−2	0.1622−1	0.5071−2	0.1641−2	0.0325−2	0.1241−1
180.0	0.2362−1	0.0223−2	0.2050−1	0.0005−2	0.1348−1	0.0251−2	0.1177−1

in surface plots of the differential cross section in Figures 3–5 for energies in the range 6.8–30.0 eV. We have studied the nature of this differential cross section in some detail, and found that destructive interference between partial-wave contributions to the scattering amplitude is responsible for the appearance of these critical angles at which the differential cross section is a minimum.

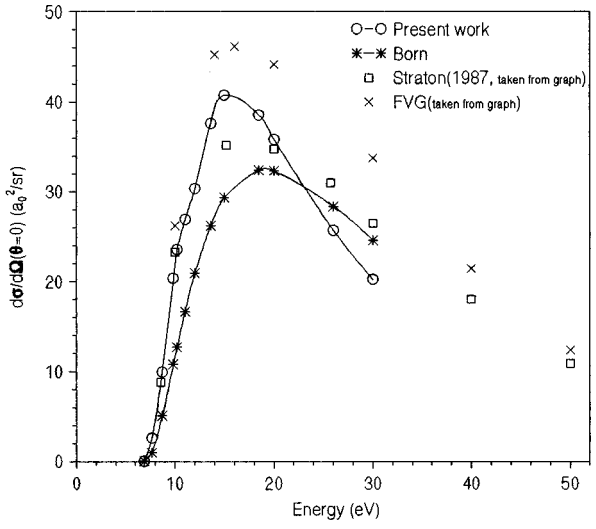

FIG. 6. Forward scattering for ground-state positronium formation in positron-hydrogen collisions in the energy range 6.8–50.0 eV.

The values of the Ps formation differential cross section are quite small at energies close to the threshold. Critical angles do, however, appear at large angles at these energies. With the increase of incident positron energy, the magnitude of the differential cross section increases with the critical angle shifting toward the forward angle. In order to visualize this aspect of the differential cross section, we have included results for positron momentum only up to 0.80 (a.u.) in Fig. 3. The first structure is related to the incident energy of the positron close to the threshold, while the appearance of critical angles is manifest as a deep gorge in the valley of the cross section along with secondary maxima at large angles, wherever these are present.

The general nature of the critical angles as a function of incident energy is as follows. At positron energies near the threshold at 6.8 eV, the Ps formation differential cross section is rather spread out, displaying a shallow minimum at a large scattering angle. As the energy increases, this angle shifts in the forward direction, with forward peaking in the cross section, given by the quantity $R=4\pi(d\sigma/d\Omega)_{\theta=0}/\sigma$. The value of R equals 1.0 for isotropic scattering. In Table II, we show the values of this quantity, along with the critical angles, the differential cross section at the forward angle 0° and at fixed angles 45°, 60°, and 120°, and the total reaction cross section as given by the

Schwinger variational method in the energy range 6.8–30.0 eV. The values of the Ps formation differential cross section are given in Table III for several positron energies 6.855 76, 8.704, 10.2, 13.6, 20.0, 26.0, and 30.0 eV.

In order to show how the present forward differential cross section compares with those obtained by other theoretical methods including the Born approximation, we further display $(d\sigma/d\Omega)_{\theta=0}$ in Fig. 6 as a function of the incident positron energy. The present values rise sharply to a peak at an incident energy of around 15 eV, where the total Ps formation cross section also reaches maximum and then fall off steadily. At low energies near the threshold, our calculation agrees with those of Straton [18] and Ficocelli, Varracchio, and Girardeau [29], but the peak value obtained by us is much higher than those predicted by other calculations. At higher energies, while the other values fall at a much slower rate, the present values fall off sharply. As is evident, the first Born values are much smaller than all other cross sections at the forward angle. The behavior of the differential cross section near the forward direction thus seems to be responsible for the large values of the total Ps formation cross section around 15 eV. In other words, the small-angle scattering of positrons needs to be accounted for properly to understand the capture process in positron-hydrogen collisions at these energies.

V. CONCLUSIONS

We have used a formulation of the Schwinger variational principle for rearrangement collisions in momentum space using correlated discrete basis sets for positron-hydrogen atom collisions in the energy range 6.8–30 eV. The results obtained with $N=8$ terms in the basis expansion for the low energies are in full accord with the available Kohn-Hulthĕn variational calculations [13] for the partial waves $L=0$, 1, and 2 in the Oré energy gap 6.8–10.2 eV. The present calculation has been performed at several positron energies in the range 6.8–30.0 eV for all partial waves $L=0-15$.

The predicted results for the total Ps formation cross section agree nicely with the observed data of Zhou *et al.* [23] over the entire energy range, as well as with the recent variational and nonvariational calculations [14,20,21]. The present calculation displays surface plots of the differential cross section and, predicts the existence of critical angles. Rich structures are revealed by this display of the surface plots. With this, a comprehensive study seems to have been performed by the present application of the Schwinger variational principle for rearrangement collisions to positron-hydrogen scattering at low-energies. Further applications of the method are in progress.

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