Positronium formation using the multichannel Schwinger variational principle

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The mutlichannel Schwinger variational formalism in the momentum space has been used to investigate elastic scattering and the ground-state positronium formation process in the positron-hydrogen collisions in the Ore gap region, 6.8–10.2 eV. The *s*-wave results obtained by employing a correlated discrete basis set are found to be in agreement with existing accurate Kohn variational results of Humberston [Can. J. Phys. **60**, 591 (1982)].

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I. INTRODUCTION

The positron-hydrogen collision system consists of a perfect three-body scattering problem, as the participating particles in the incident channel, positron +(electron+proton), are all distinct. Because of the simplicity of the system, as the bound-state wave functions are exactly known, quite a number of theoretical scientists have paid attention to the problem. And now, with the advent of new technological breakthroughs, reports of observations of the cross sections for the elastic scattering, impact excitation, ionization, and positronium (Ps) formation in the laboratory are forthcoming [1,2]. This has imparted a further impetus in the activities of positron research these days.

In the incident energy region below the Ps formation threshold at 6.8 eV, the scattering problem may be considered to be solved. Calculations of various degrees of sophistication have been performed by employing a wide class of approximation schemes over the years. Most notable among them are those reported by using the Kohn-Hulthén variational method [3–14], the coupled-static-plus correlations (CSC) approximation [15,16], the complex-coordinate-rotation (CCR) method [17], the moment T-matrix extrapolation method [18], a new version of the R-matrix method [19], and the Schwinger variational principle [20–22]. Many variants of the close-coupling approximations (CCA's) with and without inclusion of excited states, pseudostates, and the virtual Ps formation effect below 6.8 eV have also been applied with encouraging results [23–27]. Furthermore, attempts have been made to study the system by considering the complete second-order adiabatic potential and also by making nonadiabatic corrections to the Callaway-Temkin polarization potential [28–31]. The most significant results for the elastic scattering *s*- and *p*-wave phase shifts, however, have been obtained by the Kohn-Hulthén lower bound calculation of Bhatia *et al.* [8,13] using a huge number of Hylleraas correlation functions, thus confirming the accuracy of the *s*-wave results reported a decade earlier by Schwartz [5]. These investigations of Bhatia *et al.* depended heavily on the minimum principles discovered by Spruch and co-workers [4,6,32–34]. Accurate results for the higher partial waves have subsequently been obtained for the *d* wave by Register and Poe [14], for partial waves $l \leq 5$ by Winick and Reinhardt [18] and for $l \leq 4$ by Higgins, Burke, and Walters [19]. The Schwinger variational phase shifts reported recently [20–22] are in conformity with these results.

Above the Ps formation threshold we face the really difficult problem of solving the scattering equations. When both elastic and Ps formation channels are open, it is from the nonorthogonality of the wave functions of hydrogen and Ps atoms that most of the troubles comes. In addition, both the atoms are polarizable, the polarizability of a Ps atom being 8 times that of hydrogen. Moreover, the repulsive static interaction acts in opposition to the adiabatic dipole polarization potential. Careful consideration of the effects arising out of these interactions are needed.

The pioneering work relating to Ps formation has been performed by Massey and Mohr [35] in which they computed the total cross sections for Ps formation in the ground state in positron-hydrogen collisions within the framework of the first Born approximation (FBA). They made limited use of the distorted-wave approximation (DWA) in order to study the effects of distorted elastic waves on the ground-state Ps formation. As expected, the distorted waves lowered the cross-section values significantly from those obtained by FBA.

During the past four decades, a host of calculations has been reported which may be broadly classified into two categories depending upon the energy E_i of the incident positron. At low energies in the Ore gap region, 6.8 eV $< E_i <$ 10.2 eV for e^+H collisions, in which only elastic scattering and Ps formation channels are open, sophisticated variational and nonvariational calculations using the Kohn-Hulthén method [12,36,37], the generalized-variational-bound (GVB) method [38], the R-matrix method [39], the coupled static approximation [25,40,41], a multistate CCA with and without pseudostates [27,42,43], the CSC approximation [15,16], the moment T-matrix approach [18], and the CCR method [17] are available.

In the intermediate- and high-energy region for E_i beyond 10.2 eV, a wide variety of approximations has been applied to predict total and differential cross sections for elastic scattering, impact excitation, ionization,

and Ps formation in the ground as well as excited states [44–52]. Particular mention may be made of the calculations on Ps formation by making use of the impulse approximation [53], the first-order Faddeev-Watson multiple-scattering approximation [54], the second-order Born approximation [55–57], the integral CCA [41,42], a class of first-order approximations including FBA [58,59], distorted-wave approximation with and without polarization effects [60–64], the field-theoretic approach [65,66], the classical trajectory Monte Carlo technique [67,68], Fock-Tani equations [69], and the eikonal-Glauber approximation [70].

In the present work we describe a formulation of the multichannel Schwinger variational principle in momentum space. In addition to the advantages of the Schwinger variational method as explored by McKoy and co-workers [71–76] in recent years, the present formulation offers an expression of the stationary K matrix which involves two-body "input" matrix elements which are rather easy to generate for any partial wave l. We have applied the single-channel version of the present formalism to compute s-, p-, d-, and higher partial-wave phase shifts for elastic positron scattering by hydrogen below the pickup threshold at 6.8 eV with encouraging results [20–22].

We make an application of the method to study one of the most interesting problems of atomic physics, namely, Ps formation in positron-hydrogen scattering at low energies below the first excitation threshold of hydrogen at 10.2 eV. In this energy region ($6.8 < E_i < 10.2$ eV), accurate results have been reported for partial waves $l \leq 2$ by making use of the Kohn-Hulthén variational method by Humberston [36], and Brown and Humberston [37] in which huge sets of Hylleraas correlation functions are utilized. One of the major innovations of the present calculation is the use of a new type of correlation function which is dependent on the interparticle coordinate $\mathbf{r}_{12}$ through an infinite order. Utility of such correlation functions in other areas of atomic and molecular physics can be ascertained only after further applications.

The plan of the paper is as follows. In Sec. II we give the formulation of the multichannel Schwinger principle in momentum space and in Sec. III describe the numerical methods for evaluation of relevant two-body and Green's-function matrix elements. The results obtained from these calculations for s-wave elastic scattering and Ps formation are discussed in Sec. IV. The concluding remarks are finally made in Sec. V. We have used atomic units throughout the work, in which $a_0 = m = \hbar = e = 1$, e^2/a_0(unit of energy)$= 27.2$ eV.

II. THEORY

We consider a two-channel scattering problem. Let the total Hamiltonian of the system be split up into channel Hamiltonians as

$$H = H_i + V_i = H_f + V_f \ , \tag{1}$$

where V_i, V_f are residual interactions in the incident and final channels, respectively.

The unperturbed plane-wave states in each channel satisfy the equations

$$H_i|\Phi_i\rangle = E_i|\Phi_i\rangle \tag{2}$$

$$H_f|\Phi_f\rangle = E_f|\Phi_f\rangle \ . \tag{3}$$

Since the total energy E of the system must be conserved for transition from state i to state f, $E = E_i = E_f$ yields

$$k_i^2/2\mu_i + \varepsilon_i = k_f^2/2\mu_f + \varepsilon_f \ , \tag{4}$$

(k_i, ε_i), (k_f, ε_f) denoting, respectively, the (wave number, eigenenergy) for states i and f, while μ_i, μ_f are the reduced masses.

The exact scattering matrix element for the transition from state i in channel α to state f in channel β can be written as

$$T_{fi}(\beta\mathbf{k}_f, \alpha\mathbf{k}_i) = \langle \Phi_f|V_f|\Psi_i^+\rangle = \langle \Psi_f^-|V_i|\Phi_i\rangle \ , \tag{5}$$

where $|\Psi_i^+\rangle$, $\langle\Psi_f^-|$ denote, respectively, the full solutions of the Lippmann-Schwinger equations satisfying outgoing-wave and incoming-wave boundary conditions, respectively.

We can similarly define the reactance K-matrix elements by replacing $|\Psi_i^+\rangle$, $\langle\Psi_f^-|$, respectively, with the principal-value solutions $|\Psi_i^p\rangle$, $\langle\Psi_f^p|$ satisfying stationary-wave boundary conditions:

$$|\Psi_i^p\rangle = |\Phi_i\rangle + G_i^p V_i|\Psi_i^p\rangle \ , \tag{6}$$

$$\langle\Psi_f^p| = \langle\Phi_f| + \langle\Psi_f^p|V_f G_f^p \ , \tag{7}$$

with the principal-value Green's function being given as

$$G_c^p = [1/(2\pi)^3] \sum_\gamma \mathrm{P}\int d\mathbf{k}''|\Phi_\gamma''\rangle\langle\Phi_\gamma''|/(E-E'') \ , \quad c = i, f \ , \tag{8}$$

where $|\Phi_\gamma\rangle$ are intermediate plane-wave states.

We thus obtained

$$K_{fi}(\beta\mathbf{k}_f, \alpha\mathbf{k}_i) = \langle\Phi_f|V_f|\Psi_i^p\rangle = \langle\Psi_f^p|V_i|\Phi_i\rangle \ . \tag{9}$$

On utilizing Eqs. (6) and (7) for $|\Phi_i\rangle$, $\langle\Phi_f|$ in Eq. (9), $K_{fi}(\beta\mathbf{k}_f, \alpha\mathbf{k}_i)$ may also be written as

$$K_{fi}(\beta\mathbf{k}_f, \alpha\mathbf{k}_i) = \langle\Psi_f^p|(1-V_f G_f)V_f|\Psi_i^p\rangle = \langle\Psi_f^p|V_i(1-G_i^p V_i)|\Psi_i^p\rangle \ . \tag{10}$$

Using Eqs. (9) and (10), a variational expression for the Schwinger functional for the K matrix may be defined as

$$[K_{fi}(\beta\mathbf{k}_f, \alpha\mathbf{k}_i)] = \langle\Psi_f^p|V_i|\Phi_i\rangle + \langle\Phi_f|V_f|\Psi_i^p\rangle - \langle\Psi_f^p|V_c - V_c G_c^p V_c|\Psi_i^p\rangle \ , \quad c = \text{either } i \text{ or } f \ . \tag{11}$$

This expression remains stationary, $\Delta[K_{fi}(\beta\mathbf{k}_f,\alpha\mathbf{k}_i)]=0$, under variations of $|\Psi_i^p\rangle\rightarrow|\Psi_i^p\rangle+|\Delta\Psi_i^p\rangle$, $\langle\Psi_f^p|\rightarrow\langle\Psi_f^p|+\langle\Delta\Psi_f^p|$, if we neglect terms of higher order in the variation.

The initial and final wave functions $|\Psi_i^p\rangle$ and $\langle\Psi_f^p|$ are then expanded in discrete basis sets of the channel as follows:

$$|\Psi_i^p\rangle=\sum_{a=1}^{2}\sum_{m=1}^{N}a_m^{(a)}|u_m^{(a)}\rangle\ , \tag{12}$$

$$\langle\Psi_f^p|=\sum_{b=1}^{2}\sum_{n=1}^{N}b_n^{(b)}\langle v_n^{(b)}|\ , \tag{13}$$

where the expansion coefficients $a_m^{(a)}$, $b_n^{(b)}$ $(m,n=1-N)$ are linear variational parameters for channel indices $a,b=1,2$.

It is now pertinent to define two-body scattering amplitudes as follows:

$$f_{fm}^{(fa)}(\beta\mathbf{k}_f,\alpha\mathbf{k}_a)=(-\mu_\beta/2\pi)\langle\Phi_f|E-H|u_m^{(a)}\rangle\ , \tag{14}$$

$$f_{ni}^{(bi)}(\beta\mathbf{k}_b,\alpha\mathbf{k}_i)=(-\mu_\beta/2\pi)\langle v_n^{(b)}|E-H|\Phi_i\rangle\ , \tag{15}$$

$$f_{nm}^{(ba)}(\beta\mathbf{k}_b,\alpha\mathbf{k}_a)=(-\mu_\beta/2\pi)\langle v_n^{(b)}|E-H|u_m^{(a)}\rangle\ , \tag{16}$$

with $\mathbf{k}_a=\mathbf{k}_1,\mathbf{k}_2$; $\mathbf{k}_b=\mathbf{k}_1,\mathbf{k}_2$; $\mathbf{k}_1=\mathbf{k}_i$; $\mathbf{k}_2=\mathbf{k}_f$, and write

$$K'_{fi}(\beta\mathbf{k}_f,\alpha\mathbf{k}_i)=-(\mu_\beta/2\pi)K_{fi}\ , \tag{17}$$

so as to obtain from Eq. (11), when using Eqs. (12)–(17),

$$[K'_{fi}]=\sum_a\sum_m a_m^{(a)}f_{fm}^{(fa)}+\sum_b\sum_n b_n^{(b)}f_{ni}^{(bi)}-\sum_{a,b}\sum_{m,n}a_m^{(a)}b_n^{(b)}D_{nm}^{(ba)}\ , \tag{18}$$

where we have defined the double-scattering matrix elements as

$$D_{nm}^{(ba)}=f_{nm}^{(ba)}(\beta\mathbf{k}_b,\alpha\mathbf{k}_a)+\sum_\gamma(1/4\pi^2\mu_\gamma)\mathrm{P}\int d\mathbf{k}''(E-E''_\gamma)^{-1}f_{n\gamma}(\beta\mathbf{k}_b,\gamma\mathbf{k}'')f_{\gamma a}(\gamma\mathbf{k}'',a\mathbf{k}_a)\ , \tag{19}$$

where μ_γ is the reduced mass of the channel γ.

After the partial-wave analysis according to the definition

$$A(\beta\mathbf{k}_f,\alpha\mathbf{k}_i)=[1/(k_ik_f)^{1/2}]\sum_{l=0}^{\infty}(2l+1)A_l(\beta k_f,\alpha k_i)P_l(\hat{\mathbf{k}}_f\cdot\hat{\mathbf{k}}_i)\ , \tag{20}$$

where $P_l(\hat{\mathbf{k}}_f\cdot\hat{\mathbf{k}}_i)$ are the Legendre polynomials of the first kind of order l, we are able to obtain the Schwinger functional in the form

$$[K_i^{(fi)}]=\sum_a\sum_m a_m^{(a)}f_{l(fm)}^{(fa)}+\sum_b\sum_n b_n^{(b)}f_{l(ni)}^{(bi)}-\sum_{a,b}\sum_{m,n}a_m^{(a)}b_n^{(b)}D_{l(nm)}^{(ab)} \tag{21}$$

with the partial-wave double-scattering elements given as

$$D_{l(nm)}^{(ba)}=f_{l(nm)}^{(ba)}+(2/\pi)\sum_\gamma P\int_0^\infty k''dk''(k_\gamma^2-k''^2)^{-1}f_{l(n\gamma)}^{(b\gamma)}(\beta k_b,\gamma k'')f_{l(n\gamma)}^{(\gamma a)}(\gamma k'',\alpha k_a)\ . \tag{22}$$

We now optimize $[K_i^{(fi)}]$ with respect to linear variational parameters $a_m^{(a)},b_n^{(b)}$:

$$\frac{\partial}{\partial a_m^{(a)}}[K_l^{(fi)}]=0=\frac{\partial}{\partial b_n^{(b)}}[K_l^{(fi)}]\ ,\qquad a=b=1,2,\ m,n=1-N\ , \tag{23}$$

and obtain these variational parameters as solutions of a set of consistent linear equations as

$$a_m^{(a)}=\sum_{b=1}^{2}\sum_{n=1}^{N}(D_{mn}^{(ab)})^{-1}f_{l(ni)}^{(bi)}\ ,\quad a=1,2,\ m=1-N\ , \tag{24}$$

$$b_n^{(b)}=\sum_{a=1}^{2}\sum_{m=1}^{N}f_{l(fm)}^{(fa)}(D_{mn}^{(ab)})^{-1}\ ,\quad b=1,2,\ n=1-N\ , \tag{25}$$

where the double-scattering matrix $D_{2N\times2N}$ is defined as

$$D_{2N\times2N}=\begin{bmatrix}D_{N\times N}^{(11)} & D_{N\times N}^{(12)}\\ D_{N\times N}^{(21)} & D_{N\times N}^{(22)}\end{bmatrix} \tag{26}$$

with the partitioning submatrices given as

$$D_{N\times N}^{(ab)}=\begin{bmatrix}D_{11}^{(ab)} & D_{12}^{(ab)} & \cdots & D_{1N}^{(ab)}\\ D_{21}^{(ab)} & D_{22}^{(ab)} & \cdots & D_{2N}^{(ab)}\\ \vdots & \vdots & \ddots & \vdots\\ D_{N1}^{(ab)} & D_{N2}^{(ab)} & \cdots & D_{NN}^{(ab)}\end{bmatrix} \tag{27}$$

having the symmetry property that $D_{N\times N}^{(12)}=D_{N\times N}^{(21)}$. The inverse of the real symmetric matrix $D_{2N\times2N}$ is denoted by $D_{2N\times2N}^{-1}$ with its elements $(D_{mn}^{(ab)})^{-1}$.

On putting the coefficients from Eqs. (24) and (25) into Eq. (21), the final expression for the Schwinger K matrix in the momentum space is obtained as

$$[K_i^{(fi)}]=\sum_{a,b}\sum_{m,n}fl_{(fm)}^{(fa)}(D_{l(mn)}^{(ab)})^{-1}f_{l(ni)}^{(bi)}\ . \tag{28}$$

One of the virtues of this expression, as mentioned earlier, is that it requires only the two-body scattering amplitudes as obtained from Eqs. (14)–(16) and (20) as input for its evaluation. Thus, for a convenient choice of the discrete basis functions, evaluation of the K matrix be-

comes rather straightforward for any partial wave l.

We apply the K matrix given by Eq. (28) to the two-channel positron-hydrogen collision reactions

$$1+(2,3)\rightarrow 1+(2,3) \quad \text{(elastic scattering)}$$
$$\rightarrow (1,2)+3 \quad \text{(Ps formation)} \tag{29}$$

in the energy region $6.8 < E_i < 10.2$ eV, in which the positron is designated as particle 1 with its position vector $\mathbf{r}_1$, and the electron as particle 2, with its position vector $\mathbf{r}_2$ referred to the proton (particle 3), which is assumed to be infinitely heavy, at the origin of the coordinate system. The relative coordinate of particles 1 and 2 is denoted as $\mathbf{r}_{12}=\mathbf{r}_1-\mathbf{r}_2$ and their center-of-mass coordinate $\mathbf{s}_{12}=(\mathbf{r}_1+\mathbf{r}_2)/2$.

In this coordinate representation, the unperturbed plane-wave states in the elastic and Ps formation channels are given by

$$\Phi_i(\mathbf{r}_1,\mathbf{r}_2)=\exp(i\mathbf{k}_i\cdot\mathbf{r}_1)\phi_i(\mathbf{r}_2) \quad \text{(incident elastic channel)} \tag{30}$$

$$\Phi_f(\mathbf{r}_1,\mathbf{r}_2)=\exp(i\mathbf{k}_f\cdot\mathbf{r}_1)\phi_f(\mathbf{r}_2) \quad \text{(scattered elastic channel)} \ (f=i,\ |\mathbf{k}_i|=|\mathbf{k}_f|)$$
$$=\exp(i\mathbf{k}_f\cdot\mathbf{s}_{12})\eta(\mathbf{r}_{12}) \quad \text{(scattered Ps formation channel)} \ (f\neq i)\ . \tag{31}$$

The propagation number k_f of the moving Ps is obtained from Eq. (4):

$$k_i^2/2\mu_i-1/2n^2=k_f^2/2\mu_f-1/4n^2 \ \text{(a.u.)}\ , \quad n=1\ , \tag{32}$$

in which the reduced mass in the elastic channel, $\mu_i=m(m+M)/\{m+(m+M)\}\rightarrow m=1$ (a.u.) as the proton mass $M\rightarrow\infty$ and the reduced mass in the Ps formation channel $\mu_f=M(m+m)/\{M+(M+M)\}\rightarrow m/2=\frac{1}{2}$ a.u.

The residual interactions V_i and V_f are given by $V_i=V_2+V_3=1/r_1-1/r_{12}$ (a.u.) and $V_f=V_1+V_2=-1/r_2+1/r_i$ (a.u.), where V_1 is the Coulomb interaction between 2 and 3, and so on. We have made use of the following choices for the discrete channel basis functions:

$$u_m^{(1)}(\mathbf{r}_1,\mathbf{r}_2)=(-1)^{m-1}\exp(-\alpha_m r_1+i\mathbf{k}_i\cdot\mathbf{r}_1-xr_{12})\phi_i(\mathbf{r}_2)/(r_{12}+a)^j \quad \text{(elastic channel)} \tag{33}$$

$$u_m^{(2)}(\mathbf{r}_1,\mathbf{r}_2)=(-1)^{m-1}\exp(-\alpha_m r_1+i\mathbf{k}_f\cdot\mathbf{s}_{12}-xr_{12})\eta(\mathbf{r}_{12})/(r_{12}+a)^j \quad \text{(Ps formation channel)}\ , \tag{34}$$

$j=1$ for $m=1,2$; $j=2$ for $m=3,4$ and so on,

where a, p, κ denote three nonlinear variational parameters which are to be optimized by exploiting the stationary property of $[K_i^{(fi)}]$ in Eq. (28), $\alpha_m=0$ or p according to whether m is odd or even. Since the asymptotic characters of the wave function is unimportant in the Schwinger variational calculation, an identical choice has also been made for the basis functions $v_n^{(b)}(\mathbf{r}_1,\mathbf{r}_2)$ $(b=1,2)$.

III. EVALUATION OF TWO-BODY AND GREEN'S-FUNCTION MATRIX ELEMENTS $\langle\Psi_f^p|V_iG_i^pV_i|\Psi_i^p\rangle$

The importance of the accurate determination of Green's-function matrix elements in atomic and molecular collision physics has been felt over the years. These matrix elements are frequently encountered among other places in the evaluation of the double-scattering term in the CCA, the second-order Born approximation (SBA), and the Schwinger variational principle. Since the full wave function is expanded in a few low-lying target bound states along with the possible inclusion of some pseudostates in the application of CCA, evaluation of the matrix elements has been performed with relative ease. In SBA, as in CCA, people usually consider a few intermediate bound states in the Green's function and then use what is known as the "closure" approximation, so that the double-scattering term is evaluated without much difficulty. However, the application of the Schwinger variational principle to atomic and molecular collision problems has not been very extensive due to the presence of these Green's-function matrix elements, because of the fact that, in this case, the basis functions are quite arbitrary and not restricted to the bound state of the target alone. For a respectable calculation one would prefer using basis functions which include, among other things, a sufficient number of correlation functions depending upon the interparticle coordinate $\mathbf{r}_{12}$. And the evaluation of these matrix elements with the possible inclusion of such a correlation is a rather difficult task which therefore discourages people from using the Schwinger variational principle even though it has other distinctive features over the Kohn-Hulthén-type variational principle, as has been shown by Lucchese, Takatsuka, and McKoy considering the same potential and the same basis functions for both the methods [75].

We consider below an efficient method of evaluation of Green's-function matrix elements in the momentum space with correlation functions as employed in the present and previous calculations [20–22]. Watson *et al.* [74] and Lima *et al.* [77] have also prescribed methods of evaluating these matrix elements in configuration and momentum spaces in which they have, however, employed uncorrelated basis functions.

For the purpose of demonstrating the method of calculation, let us assume that only elastic scattering is possible, so that $a=1$, $b=1$, $N=1$, $f=i$. We consider the double-scattering matrix element involving the Green's function,

$$\mathcal{D}_{nm}^{(11)}=(-\mu/2\pi)\langle v_n^{(b)}|V_iG_i^pV_i|u_m^{(a)}\rangle\ , \tag{35}$$

and assume that the summation index includes only the ground state i of the intermediate discrete bound states.

Then the two-body scattering amplitudes given by Eqs. (14)–(16) take the form

$$f_{fm}^{(f1)}(\alpha\mathbf{k}_f,\alpha\mathbf{k}_i)=(-\mu_f/2\pi)\langle\Phi_f|E-H|u_m^{(1)}\rangle$$
$$=-(\mu_f/2\pi)[\langle\Phi_f|V_i|u_m^{(1)}\rangle+(E_f-E_m)\langle\Phi_f|u_m^{(1)}\rangle]$$
$$=f_{fm}^{(f1)}(\text{on shell})+f_{fm}^{(f1)}(\text{off shell}) , \tag{36}$$

$$f_{ni}^{(1i)}(\alpha\mathbf{k}_f,\alpha\mathbf{k}_i)=(-\mu_f/2\pi)\langle v_n^{(1)}|E-H|\Phi_i\rangle$$
$$=(-\mu_f/2\pi)[\langle v_n^1|V_i|\Phi_i\rangle+(E_n-E_i)\langle v_n^{(1)}|\Phi_i\rangle]$$
$$=f_{ni}^{(1i)}(\text{on shell})+f_{ni}^{(1i)}(\text{off shell}) . \tag{37}$$

It should be mentioned that, for energy-conserving transitions, the off-shell contributions would become zero, as either $E_f=E_m$ or $E_n=E_i$.

After performing the partial-wave analysis, the Green's-function matrix element takes the final form:

$$\mathcal{D}_{l(nm)}^{(11)}=(2/\pi)\mathrm{P}\int_0^\infty k''dk''(k_i^2-k''^2)^{-1}f_{l(ni)}(\alpha k_f,\alpha k'')f_{l(im)}(\alpha k'',\alpha k_i) , \tag{38}$$

in which the two-body amplitudes are to be supplied and the symbol P stands for the principal value of the improper integral. The single-dimensional principal-value integral over $[0,\infty)$ is carried out numerically by breaking it up into two integrals over $[0,2k_i]$ and $[2k_i,\infty)$:

$$\mathrm{P}\int_0^\infty\cdots=\mathrm{P}\int_0^{2k_i}\cdots+\int_{2k_i}^\infty\cdots , \tag{39}$$

in which the second integral is an improper integral in the Cauchy-Riemann sense. We are to evaluate the principal-value integral over $[0,2k_i]$ by using an even number of Gauss-Legendre quadrature points so as to distribute the mesh points symmetrically around the midpoints k_i. In this way the definition of a principal-value integral,

$$\mathrm{P}\int_0^{2k_i}\cdots=\lim_{\epsilon\to0}\left[\int_0^{k_i-\epsilon}\cdots+\int_{k_i+\epsilon}^{2k_i}\cdots\right] , \tag{40}$$

is satisfied numerically since, as the number of quadrature points was increased, the nearest points around k_i would be progressively approaching k_i from both sides at the same rate. The other integral on $[2k_i,\infty)$ is easily performed by using either the Gauss-Legendre or the Gauss-Laguerre quadrature method after suitable transformation of the integration variable.

On using the basis functions (33) in Eqs. (36) and (37), the required two-body amplitudes are obtained. The expression for the on-the-energy-shell scattering amplitudes $f_{ni}^{(1i)}(\alpha\mathbf{k}_f,\alpha\mathbf{k}_i)$ takes the form

$$f_{ni}^{(1i)}(\text{on shell})=N_1\int d\mathbf{r}_1d\mathbf{r}_2\exp(i\boldsymbol{\Delta}\cdot\mathbf{r}_1-\alpha_nr_1-xr_{12}-\lambda_ir_2)(1/r_1-1/r_{12})/(r_{12}+a)^n ,$$
$$\alpha_{2n-1}=0,\ \alpha_{2n}=p\ ,\ n=1,N\ , \tag{41}$$

where the overall constant $N_1=(-\mu_f/2\pi)(\lambda_i^{3/2}/\sqrt{\pi})(-1)^{n-1}$, $\lambda_i=1/a_0=1$ (a.u.), with the momentum transfer vector $\boldsymbol{\Delta}=\mathbf{k}_i-\mathbf{k}_f$. The functional dependence is separated into coordinates $\mathbf{r}_1$ and $\mathbf{r}_2$ by first taking the Laplace transform of $1/(r_{12}+a)^n$ and then integrating over $d\mathbf{r}_1$ and $d\mathbf{r}_2$ by using Fourier integral transforms along with δ-function properties. We obtain

$$f_{ni}^{(1i)}(\text{on shell})=C_1\int_0^\infty\exp(-at)t^{n-1}dt[(n-1)!]^{-1}\left[\tau\int d\mathbf{s}/[(s^2+\tau^2)^2(s^2+\beta^2)^2(|\mathbf{s}+\boldsymbol{\Delta}|^2+\alpha_n^2)]\right.$$
$$\left.-\alpha_n\int d\mathbf{s}/[(s^2+\tau^2)(s^2+\beta^2)^2(|\mathbf{s}+\boldsymbol{\Delta}|^2+\alpha_n^2)^2]\right] , \tag{42}$$

where $C_1=-16\mu_f\beta\lambda_i^3(-1)^{n-1}$, $\beta=2\lambda_i$, $\mu_f=1$.

The residual volume integration over $d\mathbf{s}$ is finally carried out by utilizing the Lewis integral [78] to yield

$$f_{ni}^{(1i)}(\text{on shell})=C_0\int_0^\infty\exp(-at)t^{n-1}dt[(n-1)!]^{-1}[\mathsf{L}^{(\tau\beta)}(\beta;-\boldsymbol{\Delta},\alpha_n;0,\tau)-\mathsf{L}^{(\beta\alpha_n)}(\beta;-\boldsymbol{\Delta},\alpha_n;0,\tau)] , \tag{43}$$

where the Lewis function $\mathsf{L}(\lambda;\mathbf{p}_1,\mu_1;\mathbf{p}_2,\mu_2)$ is defined by

$$\mathsf{L}(\lambda;\mathbf{p}_1,\mu_1;\mathbf{p}_2,\mu_2)=(1/\pi^2)\int d\mathbf{s}/[(s^2+\lambda^2)(|\mathbf{s}-\mathbf{p}_1|^2+\mu_1^2)(|\mathbf{s}-\mathbf{p}_2|^2+\mu_2^2)] \tag{44}$$

with its derivatives $\mathsf{L}^{(\tau\beta)}$, $\mathsf{L}^{(\beta\alpha_n)}$ given with respect to the parameters τ,β and β,α_n, respectively. Here $C_0=-8\mu_f\lambda_i^3$.

The partial-wave form of the on-shell amplitude is obtained by performing a further integration over $d(\cos\theta)$, $\hat{\mathbf{k}}_f\cdot\hat{\mathbf{k}}_i=\cos\theta$ as in Eq. (20), by the Gauss-Legendre quadrature method:

TABLE I. Convergence of the double-scattering terms $\mathcal{D}_{l(nm)}^{(11)}$ for increasing Gauss-Legendre quadrature points at an incident positron momentum $k_i=0.8$ a.u. for the set of nonlinear variational parameters $p=0.5$, $a=0.1$, and $\kappa=0.1$. The numbers in brackets give the multiplicative powers of 10.

Gauss-Legendre quadrature points	$\mathcal{D}_{l(11)}^{(11)}$	$\mathcal{D}_{l(12)}^{(11)}$	$\mathcal{D}_{l(13)}^{(11)}$	$\mathcal{D}_{l(14)}^{(11)}$
12	0.1047	−0.4474[−1]	0.3707	−0.1940
16	0.1048	−0.4470[−1]	0.3722	−0.1945
20	0.1049	−0.4469[−1]	0.3725	−0.1947
24	0.1049	−0.4469[−1]	0.3725	−0.1947

$$f_{l(ni)}^{(1i)}(\text{on shell})=[(k_f k_i)^{1/2}/2]C_0\int_{-1}^{+1} f_{ni}^{(1i)}(\text{on shell})P_l(\cos\theta)d(\cos\theta)\ , \tag{45}$$

where θ is the scattering angle.

The off-the-energy-shell amplitudes as given by $f_{ni}^{(1i)}$ (off shell) in Eq. (37) can be evaluated in an identical manner. After the partial-wave analysis, these amplitudes are obtained as

TABLE II. The values of the on-shell amplitudes $f_{(ni)}^{(1i)}$ (on-shell) from Eq. (43) as a function of the scattering angle at incident positron momentum $k_i=0.6$ a.u. for nonlinear variational parameters $a=1.8$, $p=0.5$, and $\kappa=0.5$. The angles correspond to 36 Gauss-Legendre quadrature points. The numbers in brackets denote powers of 10.

	Angle (deg)	$f_{(1i)}^{(1i)}$	$f_{(2i)}^{(1i)}$	$f_{(3i)}^{(1i)}$	$f_{(4i)}^{(1i)}$
1	3.775	0.2166	0.2884[−1]	0.8540[−1]	0.1902[−1]
2	8.665	0.2127	0.2835[−1]	0.8438[−1]	0.1884[−1]
3	13.584	0.2060	0.2748[−1]	0.8258[−1]	0.1853[−1]
4	18.509	0.1967	0.2625[−1]	0.8009[−1]	0.1810[−1]
5	23.437	0.1855	0.2471[−1]	0.7699[−1]	0.1754[−1]
6	28.366	0.1728	0.2288[−1]	0.7340[−1]	0.1688[−1]
7	33.296	0.1591	0.2082[−1]	0.6942[−1]	0.1613[−1]
8	38.226	0.1448	0.1857[−1]	0.6519[−1]	0.1530[−1]
9	43.156	0.1305	0.1618[−1]	0.6079[−1]	0.1441[−1]
10	48.087	0.1163	0.1370[−1]	0.5633[−1]	0.1348[−1]
11	53.018	0.1026	0.1117[−1]	0.5188[−1]	0.1251[−1]
12	57.949	0.8955[−1]	0.8636[−2]	0.4753[−1]	0.1154[−1]
13	62.879	0.7724[−1]	0.6126[−2]	0.4331[−1]	0.1055[−1]
14	67.810	0.6576[−1]	0.3671[−2]	0.3927[−1]	0.9581[−2]
15	72.741	0.5516[−1]	0.1296[−2]	0.3545[−1]	0.8628[−2]
16	77.672	0.4545[−1]	−0.9786[−3]	0.3186[−1]	0.7702[−2]
17	82.603	0.3661[−1]	−0.3139[−2]	0.2851[−1]	0.6809[−2]
18	87.534	0.2861[−1]	−0.5175[−2]	0.2541[−1]	0.5957[−2]
19	92.466	0.2141[−1]	−0.7079[−2]	0.2255[−1]	0.5148[−2]
20	97.397	0.1495[−1]	−0.8849[−2]	0.1994[−1]	0.4387[−2]
21	102.328	0.9196[−2]	−0.1048[−1]	0.1756[−1]	0.3674[−2]
22	107.259	0.4081[−2]	−0.1198[−1]	0.1541[−1]	0.3011[−2]
23	112.190	−0.4448[−3]	−0.1335[−1]	0.1347[−1]	0.2398[−2]
24	117.121	−0.4433[−2]	−0.1459[−1]	0.1172[−1]	0.1836[−2]
25	122.051	−0.7934[−2]	−0.1571[−1]	0.1017[−1]	0.1323[−2]
26	126.982	−0.1099[−1]	−0.1671[−1]	0.8788[−2]	0.8580[−3]
27	131.913	−0.1365[−1]	−0.1759[−1]	0.7571[−2]	0.4407[−3]
28	136.844	−0.1594[−1]	−0.1838[−1]	0.6507[−2]	0.6943[−4]
29	141.774	−0.1790[−1]	−0.1906[−1]	0.5584[−2]	−0.2573[−3]
30	146.704	−0.1955[−1]	−0.1964[−1]	0.4794[−2]	−0.5407[−3]
31	151.634	−0.2094[−1]	−0.2014[−1]	0.4129[−2]	−0.7822[−3]
32	156.563	−0.2206[−1]	−0.2055[−1]	0.3582[−2]	−0.9830[−3]
33	161.491	−0.2295[−1]	−0.2088[−1]	0.3146[−2]	−0.1144[−2]
34	166.416	−0.2362[−1]	−0.2112[−1]	0.2818[−2]	−0.1266[−2]
35	171.335	−0.2407[−1]	−0.2129[−1]	0.2593[−2]	−0.1351[−2]
36	176.225	−0.2432[−1]	−0.2139[−1]	0.2468[−2]	−0.1397[−2]

$$f^{(1i)}_{l(ni)}(\text{off shell})=[(k_i k_f)^{1/2}/2]C_2\int_{-1}^{+1}P_l(\cos\theta)\left[\int_0^{\infty}\exp(-at)t^{n-1}dt[(n-1)!]^{-1}L^{(\tau\beta\alpha_n)}(\beta;-\Delta,\alpha_n;0,\tau)\right]d(\cos\theta)\ , \quad (46)$$

where $C_2=2\mu_f(E-E'')$.

Thus finally the scattering amplitudes $f^{(1i)}_{l(ni)}(\alpha k_f,\alpha k'')$ for the partial wave l is given as a sum of the on-shell and off-shell contributions

$$f^{(1i)}_{l(ni)}=f^{(1i)}_{l(ni)}(\text{on shell})+f^{(1i)}_{l(ni)}(\text{off shell})\ . \quad (47)$$

The remaining partial-wave amplitudes $f^{(i1)}_{l(im)}(\alpha k'',\alpha k_i)$ in the expression of $\mathcal{D}^{(11)}_{l(nm)}$ may be obtained similarly. In fact, for elastic collisions the scattering amplitudes $f^{(1i)}_{l(ni)}$ and $f^{(i1)}_{l(im)}$ are identical in form to our choice of basis functions (33).

Computation of the values of the required matrix elements $\mathcal{D}^{(11)}_{l(mn)}$ as a function of the incident momentum k_i is next done for any partial wave l without any difficulty for basis indices $m,n=1-N$. The results indicate that the convergence of these matrix elements are smooth, as shown in Table I. The "input" scattering amplitudes $f^{(1i)}_{l(ni)}$ and $f^{(i1)}_{l(im)}$ are each evaluated numerically by using energy-dependent transformation and splitting the t integral over $[0,\infty)$ into two integrals on $[0,b_n]$ and $[b_n,310.0]$, where $b_n=0.6$ for $n=1,2$ and $b_n=5.0$ for $n=3,4$. This is done to accommodate the highly peaking nature of the integrand near $t=0$ when either m or $n=1$. The integrations are then carried out by using the Gauss-Legendre method with 24 mesh points. The angle integration over $\cos\theta\varepsilon[-1,+1]$ is performed by the same method using 20 quadrature points. The results have been tested with a lesser number of quadrature points in order to achieve the convergence.

In Table II, we have shown the detailed nature of the values of the two-body on-shell amplitudes $f^{(1i)}_{ni}$ (on shell) given by Eq. (43) as a function of the scattering angle θ for a single positron momentum $k_i=0.6$. It is found that in the amplitudes for $n=1,2,4$ the contributions from the interactions $1/r_1$ and $-1/r_{12}$ tend to cancel each other out at an intermediate scattering angle which depends on the incident momentum k_i as well as on the variational parameters a, p, and κ. This feature of the two-body scattering amplitude becoming zero at some scattering angle is also manifested by the FBA amplitude for Ps formation in positron-atom collisions [58,59,61]. It is thus believed that a fair amount of attractive interaction due to virtual Ps formation is taken care of by these two-body amplitudes in predicting accurate results of elastic positron scattering by hydrogen below the Ps formation threshold [20–22]. It has been observed in these calculations that useful predictions can be made by considering only a few terms in the correlated basis set. A point worth mentioning is that only four terms were found to be sufficient in obtaining the elastic phase shifts below the pickup threshold for all the partial waves $l=0$, 1, 2, 3, . . . , L, where $L=12$ at most for the highest positron energy 6.6640 eV corresponding to $k_i=0.7$ (a.u.), very close to the threshold.

IV. RESULTS AND DISCUSSION

We have made use of Eq. (28) to compute the s-wave Schwinger K matrices K_{11}, K_{12} $(=K_{21})$, and K_{22} for three incident positron energies in the Ore gap region and have compared them with the existing results available in the literature. In optimizing the nonlinear variational parameters a, p, κ involved in the expression of the stationary κ matrix, we have adopted the following procedure. For a given value of the variational parameter a, we fix κ and compute $[K_l^{(fi)}]$ for several values of p in the range of 0.1–4.0 at a step size of 0.1 or 0.2. Then for small

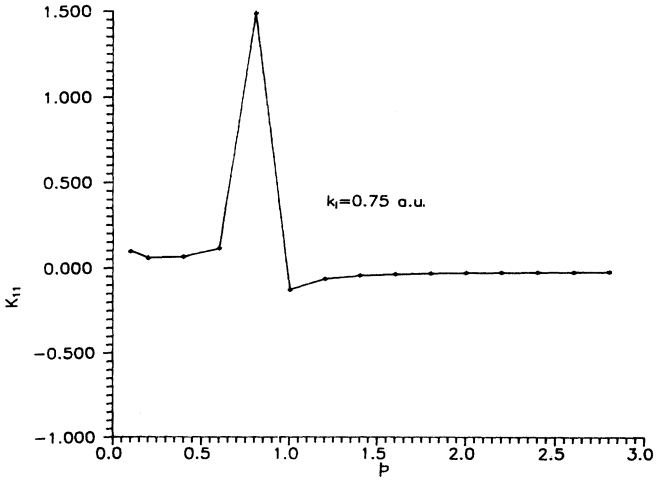

FIG. 1. The elastic scattering reactance matrix K_{11} as a function of the nonlinear variational parameter p for $a=0.55$ and $\kappa=3.5$ at an incident positron momentum $k_i=0.75$ a.u.

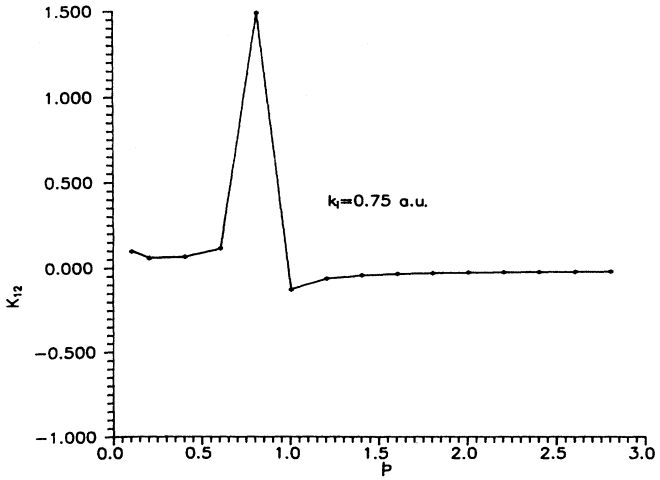

FIG. 2. The Ps formation reactance matrix K_{12} as a function of the nonlinear variational parameter p for $a=0.55$ and $\kappa=3.5$ at positron momentum $k_i=0.75$ a.u.

TABLE III. Results of K-matrix elements for incident momenta k_i in the Ore gap region. The Schwinger stationary values are obtained for the same nonlinear variational parameter $a=0.55$ at all energies E_i. The numbers in parentheses denote the uncertainty in the last digits.

k_i (a.u.)	E_i (eV)	K_{11}	K_{12}	p	κ
0.75	7.650	−0.078(7)[a]	−0.023(2)[a]	2.4	3.5
		−0.078[b]	−0.028[b]		
		−0.0862[c]	−0.025[c]		
		−0.133[d]	−0.0027[d]		
		−0.323[e]	−0.0025[e]		
		−0.233[f]	−0.0007[f]		
0.80	8.704	−0.169(5)[a]	−0.052(3)[a]	2.4	2.0
		−0.104[b]	−0.051[b]		
		−0.111[c]	−0.047[c]		
		−0.159[d]	−0.0087[d]		
		−0.347[e]	−0.035[e]		
		−0.257[f]	−0.0051[f]		
		−0.105[g]	−0.050[g]		
0.85	9.826	−0.277(22)[a]	−0.115[a]	1.8	1.25
		−0.130[b]	−0.126[b]		
		−0.137[c]	−0.132[c]		
		−0.185[d]	−0.105[d]		
		−0.367[e]	−0.104[e]		
		−0.280[f]	−0.0256[f]		

[a]Present calculation.
[b]Humberston [36].
[c]Chan and Fraser [15].
[d]Dirks and Hahn [38].
[e]Coupled static.
[f]Wakid and LaBahn [1972, their approximation (e)] [28].
[g]Stein and Sternlicht (1972) [12].

changes in the variational parameter κ and fixed a, we reevaluate the K matrices for the same set of p and see if these values of $[K_l^{(fi)}]$ do exhibit any stationary range as a function of p. We repeat this procedure with small changes in the variational parameters a and κ until a suitable combination is obtained which leaves the Schwinger K matrices stationary as a function of the nonlinear variational parameter p. Efforts have been made to optimize $[K_l^{(11)}]$, $K_l^{(12)}]$, and $[K_l^{(22)}]$ with the same set of the nonlinear variational parameters a, p, and κ. It has been possible to obtain the stationary K matrices for the same value $a=0.55$. Only four terms in the basis set are sufficient to obtain meaningful results for the elastic scattering and Ps formation channels. Figures 1–4 display the nature of convergence of K_{11} and K_{12} with the variation of p for $N=4$ at positron momenta $k_i=0.75$ and 0.80 a.u. We have observed that, outside the combination of a and κ for which K_{11} and K_{12} remain stationary (as shown in these figures), the results exhibit wild variations as a function of p. Gradual changes to-

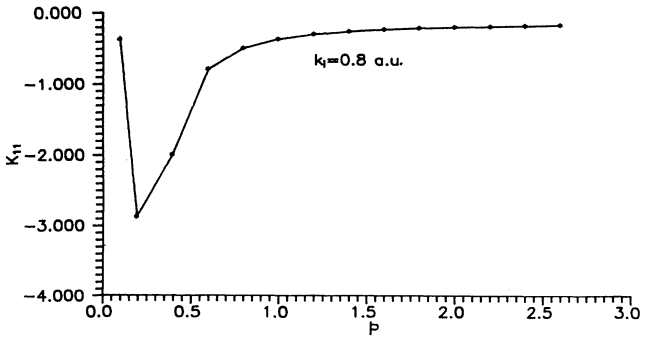

FIG. 3. Same as in Fig. 1, but for $\kappa=2.0$ at $k_i=0.80$ a.u.

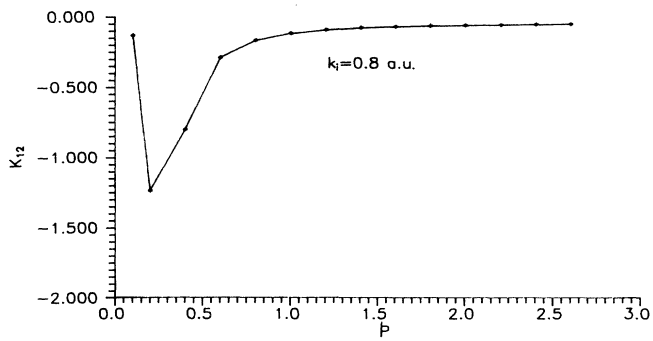

FIG. 4. Same as in Fig. 2, but for $\kappa=2.0$ at $k_i=0.80$ a.u.

wards the suitable combination of these variational parameters make the K matrices steadier and steadier.

In Table III we show the present values of K_{11} and K_{12} along with the results of Humberston [36], Dirks and Hahn [38], Chan and Fraser [15], Stein and Sternlicht [12], and Wakid and LaBahn [28]. We find that Schwinger s-wave results are in close agreement with Kohn variational results obtained by Humberston [36].

There is, however, reason to believe that there is a further scope of improvement of the present results by using basis wave functions that take full account of electron-positron correlations as well as polarization effects, particularly in the Ps formation channel. This is because of the fact that the values of the reactance matrix K_{22} as obtained in the present calculation are small and not fully converged while the other two K matrices are stationary in the same range of p (see Figs. 1–4).

One of the possible ways of improving the present basis functions is to include multiplicative terms of the form $(r_1+r_1^2/2)$ in Eqs. (33) and (34). In that case, however, calculations become prohibitively expensive compared to what we have achieved. An attempt has already been made to study the elastic d- and higher partial-wave phase shifts in positron-hydrogen atom collisions below 6.8 eV using Schwinger's principle with the help of a simpler version of the above function [22].

V. CONCLUSIONS

In this paper, we have presented a formulation of the multichannel Schwinger principle in the momentum space. An application of this formalism has been made to the problem of low-energy Ps formation in positron-hydrogen collisions. Utilizing a set of correlated discrete basis functions as used earlier by the authors [20–22], it has been possible to report s-wave results for the reactance matrices K_{11} and K_{12} which are in close agreement with the accurate results of Humberston [36] who used the multichannel Kohn variational method with the Hylleraas type of correlation functions.

It should be mentioned that collision studies involving many-electron systems and many-body structure calculations are being performed these days with the inclusion of mostly Hylleraas-type correlation functions with amazing accuracy. Particular mention may be made of the studies on the ground state of Ps^- by Bhatia and Drachman [79], Ho [80], and Frolov and Yeremin [81], on the doubly excited states of Ps^- by Ho [82], on the positron-hydrogen molecule collisions by Armour [83,84], on the positronium molecule Ps_2 by Ho [85], and on the resonances in positron-hydrogen atom collisions by Bhatia and Drachman [86].

It is hoped that the correlated basis functions as reported in this calculation would be found useful in many-body structure calculations and collision problems involving many-electron atomic and molecular target systems. One of the attractive features of these basis functions is that they can be generated quite easily to higher orders through the Laplace integral transforms. Instead of performing the recursion relations one has thus to evaluate definite integrals in order to get these higher-order terms. The present paper shows the method of evaluation of integrals which are rather smoothly convergent for positive integral values of m,n.

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