Positron-hydrogen scattering using an integral approach

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The positron-hydrogen collision problem has been investigated using an integral form of the close-coupling approximation for a wider range of energies. The present formalism takes care of the rearrangement channel. The effects of the excited states of both the hydrogen and positronium atoms have been neglected. The elastic and the positronium-formation cross sections have been obtained explicitly in the energy region 0–200 eV. Because the integral form was used, the two-state results are reliable. The present results differ from the first Born results even at 200 eV.

I. INTRODUCTION

In a previous paper, Banerji *et al.*[1] investigated the positron-hydrogen collision problem above the positronium (Ps)-formation threshold, taking into account both the direct and rearrangement channels. In their work they have applied an approximate form of the Faddeev equations[2] as used by Sloan and Moore[3] in which the off-shell contribution, which is of vital importance in the low-energy region, has been neglected. Further, this method cannot be employed to calculate the elastic-scattering cross sections including the coupling effect of the rearrangement channel in the energy region below the Ps-formation threshold.

In the present work these deficiencies have been removed. We have applied an integral form of the close-coupling approximation as used by Ghosh and Basu[4] and Chaudhuri *et al.*[5] The advantages of the integral form over the conventional close-coupling method[6,7] have been discussed in their works. Chaudhuri *et al.*[5] have obtained encouraging results for the electron-hydrogen problem by taking into account the exchange effect. Ghosh and Basu[4] have neglected the rearrangement channels in their calculation for the positron-hydrogen problem. Hence it seems worthwhile to investigate the same problem incorporating the Ps-formation channel. Only a few theoretical investigations on the positron-hydrogen system have been carried out with the inclusion of the Ps-formation channel.

Cody *et al.*[8] have applied the close-coupling approximation as suggested by Smith *et al.*[9] to study this problem for incident energies below the Ps-formation threshold. They retained the ground state of both the hydrogen and Ps atoms in their calculations. They have given the results for the elastic s-wave phase shift including the effect of virtual Ps formation.

This two-state close-coupling method has also been employed by Bransden and Jundi[10] (denoted by them as model A). They also made the calculations[10] using the approximate polarized-orbital method in which the effect of long-range dipole polarization has been included. They obtained the elastic as well as Ps-formation cross sections for the partial waves $l = 0$, 1, and 2 for the incident positron energy range 6.8–13.6 eV.

It is well known[11] that the results of the two-state calculations[8] for the s-wave phase-shifts in the low incident energies are not at all reliable. The importance of the Ps-formation channel in the e^+-H collision problem was first pointed out by Massey and Mohr.[12] The exact behavior of the Ps-formation cross sections has not been settled. Different workers[1,10-15] have obtained contradictory results. Moreover, Chan and Fraser[13] and Dirks and Hahn[15] have shown explicitly that the two-state results below the excitation threshold of the hydrogen atom will be changed considerably by including the short-range distortion effects. In their variational calculations, they have included those effects through suitable trial wave functions.

Here we have employed the two-state close-coupling approximation to investigate e^+-H scattering. We have calculated the cross sections up to an incident energy of 200 eV using the integral form of the close-coupling approximation. Recently, in an attempt to study the s-wave scattering of positrons by hydrogen atoms, Chan and Fraser[13] have used integral equations in the configuration space. Owing to the presence of the sine and cosine functions in their kernel, a large number of quadrature points are required in their calculations for convergent results. In our integral form of the close-coupling approximation which is in momentum space, this difficulty has not been encountered. Results for a wider energy range have been obtained without much difficulty.

The purposes of the present paper are twofold.

First of all we are interested in getting the results for e^+-H scattering at intermediate and high energies. Secondly, we wish to test the suitability and accuracy of the technique of solution. There are very few calculations beyond 13.6 eV in which the effect of Ps formation are included. Moreover, the validity of the first Born approximation has been questioned by different workers[1,5,16] for $e^{\mp}$-H scattering. This two-state approximation, which may not be suitable for predicting the s-wave phase shifts, may be helpful in determining the high-energy behavior.

II. THEORY

Let the particles 1 and 2 be the positron and the electron respectively and particle 3, the proton. We assume that the center of mass lies with the proton. The interacting potentials $V_{\alpha\beta}$ (in atomic units) are expressed as

$$V_{13}=\frac{1}{r_1}, \quad V_{23}=-\frac{1}{r_2}, \quad V_{12}=-\frac{1}{|\vec{r}_1-\vec{r}_2|}.$$

On retaining only the ground state of both the atoms, the integral form of the close-coupling equations may be expressed as[9,10]

$$\langle \vec{k}_1' 1s \mid Y_{11} \mid \vec{k}_1 1s\rangle = \langle \vec{k}_1' 1s \mid Y_{11}^B \mid \vec{k}_1 1s\rangle + \int d\vec{k}_1'' \frac{\langle \vec{k}_1' 1s \mid Y_{11}^B \mid \vec{k}_1'' 1s\rangle \langle \vec{k}_1'' 1s \mid Y_{11} \mid \vec{k}_1 1s\rangle}{E-E_1''} + \int d\vec{k}_3'' \frac{\langle \vec{k}_1' 1s \mid Y_{13}^B \mid \vec{k}_3'' \mathrm{Ps}\rangle \langle \vec{k}_3'' \mathrm{Ps} \mid Y_{31} \mid \vec{k}_1 1s\rangle}{E-E_3''}, \tag{1}$$

$$\langle \vec{k}_3' \mathrm{Ps} \mid Y_{31} \mid \vec{k}_1 1s\rangle = \langle \vec{k}_3' \mathrm{Ps} \mid Y_{31}^B \mid \vec{k}_1 1s\rangle + \int d\vec{k}_1'' \frac{\langle \vec{k}_3' \mathrm{Ps} \mid Y_{31}^B \mid \vec{k}_1'' 1s\rangle \langle \vec{k}_1'' 1s \mid Y_{11} \mid \vec{k}_1 1s\rangle}{E-E_1''}, \tag{2}$$

where 1s and Ps stand for the ground state of the hydrogen and positronium atoms, respectively. The matrix elements of the potential operators Y_{11}^B and Y_{31}^B have the form

$$\langle \vec{k}_1' 1s \mid Y_{11}^B \mid \vec{k}_1 1s\rangle = \frac{1}{8\pi^3} \int e^{-i\vec{k}_1'\cdot\vec{r}_1} \phi_{1s}(V_{13}+V_{12})\phi_{1s} e^{i\vec{k}_1\cdot\vec{r}_1} d\vec{r}_1\, d\vec{r}_2 \tag{3}$$

and

$$\langle \vec{k}_3' \mathrm{Ps} \mid Y_{31}^B \mid \vec{k}_1 1s\rangle = \frac{1}{8\pi^3} \int e^{-i\vec{k}_3'\cdot(\vec{r}_1+\vec{r}_2)/2} \phi_{\mathrm{Ps}}(H-E)\phi_{1s} e^{i\vec{k}_1\cdot\vec{r}_1} d\vec{r}_1\, d\vec{r}_2, \tag{4}$$

where ϕ_{1s} and ϕ_{Ps} are the ground-state wave functions of hydrogen and positronium atoms and $\vec{k}_1$, $\vec{k}_1'$, and $\vec{k}_3'$ are the momenta of the incident positron, scattered positron, and moving positronium respectively. It may be mentioned that the matrix element $\langle \vec{k}_3' \mathrm{Ps} \mid Y_{33}^B \mid \vec{k}_3 \mathrm{Ps}\rangle$ vanishes ($Y_{33}^B = V_{13}+V_{23}$) as expected.

The pole term in the kernel splits into two parts, viz. a δ-function part and a principal-value part (denoted as P). After the partial-wave analysis the two equations (1) and (2) reduce to

$$f_l(k_1', k_1) = f_l^B(k_1', k_1) + i f_l^B(k_1', k_1) f(k_1, k_1) + i g_l^B(k_1', k_3') g_l(k_3', k_1) - \frac{2}{\pi} \mathrm{P} \int \frac{k_1''^2\, dk_1''}{k_1^2 - k_1''^2} f_l^B(k_1', k_1'') f_l(k_1'', k_1) - \frac{2}{\pi} \mathrm{P} \int \frac{k_3''^2\, dk_3''}{k_3'^2 - k_3''^2} g_l^B(k_1', k_3'') g_l(k_3'', k_1), \tag{5}$$

$$g_l(k_3', k_1) = g_l(k_3', k_1) + i g_l^B(k_3', k_1) f_l(k_1, k_1) - \frac{2}{\pi} \mathrm{P} \int \frac{k_1''^2\, dk_1''}{k_1^2 - k_1''^2} g_l^B(k_3', k_1'') f_l(k_1'', k_1), \tag{6}$$

with

$$\langle \vec{k}_1' 1s \mid Y_{11}^B \mid \vec{k}_1 1s\rangle = -\frac{1}{4\pi^2 \mu_1} \sum_{l=0}^{\infty} \frac{2l+1}{\sqrt{k_1' k_1}} f_l^B(k_1', k_1) P_l(\hat{k}_1' \cdot \hat{k}_1), \tag{7}$$

$$\langle \vec{k}_3' \mathrm{Ps} \mid Y_{31}^B \mid \vec{k}_1 1s\rangle = -\frac{1}{4\pi^2 \mu_3} \sum_{l=0}^{\infty} \frac{2l+1}{\sqrt{k_3' k_1}} g_l^B(k_3', k_1) P_l(\hat{k}_3' \cdot \hat{k}_1), \tag{8}$$

and similar expressions for the unknown amplitudes. Here μ_α is the reduced mass of the system in the channel α.

It may be mentioned that Banerji *et al.*,[1] who have used an approximate form of the Faddeev equations, have solved two equations which are identical to Eqs. (5) and (6) neglecting the principal-value parts. One

TABLE I. Phase shifts ($l = 0$) for elastic scattering of positrons by hydrogen atoms.

k_1 (a_0^{-1})	Present	Bransden and Jundi[10] (model A)	Cody *et al.*[8]
0.7	−0.292	−0.29	−0.286
0.6	−0.242	−0.24	−0.238
0.5	−0.188	−0.20	−0.186
0.4	−0.135	−0.15	−0.134

can obtain the expression for f_l^B very easily, and the analytical expression for g_l^B has been derived in the Appendix.

The differential cross sections $d\sigma/d\Omega$ and the total cross sections σ may be obtained from the standard relations.

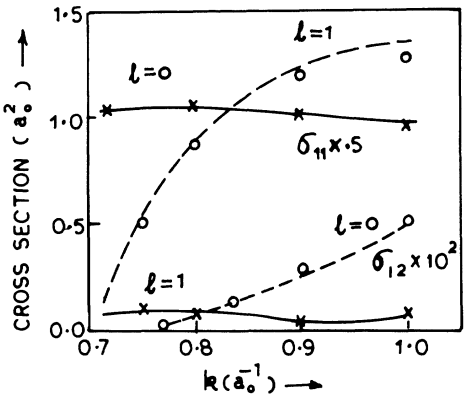

FIG. 1. Partial-wave cross section for $l = 0$ and 1. Solid lines stand for the elastic cross section and crosses are the corresponding results of Bransden and Jundi. Dashed lines represent the Ps-formation cross sections and the corresponding results of Bransden and Jundi are given by open circles.

III. RESULTS AND DISCUSSION

The coupled integral equations (5) and (6) have been solved numerically for each value of the angular momentum l. The details of the method of solution have been given by Ghosh and Basu[4] and Chaudhuri *et al.*[5]

Table I includes the s-wave phase shifts obtained by the present calculations, Cody *et al.*,[8] and Bransden and Jundi[10] (Model A) below the Ps-formation threshold. All of these phase shifts given in the table have the same sign. Our calculated phase shifts are very close to the previous calculations. Figure 1 represents the elastic and Ps-formation cross sections from 7 to 13.6 eV for $l = 0$ and 1 along with the corresponding results (Model A) of Bransden and Jundi. At 13.6 eV, our results differ from Bransden and Jundi slightly in both the channels. It may be mentioned that the s-wave Ps-formation cross section of Bransden and Jundi (curve A of Fig. 4 of their paper) is mislabeled by a factor of 10 (the results should be multiplied by 10^2 instead of 10^3). This can be found by comparing it with the results of Dirks and Hahn.[15] The present results for the partial ($l = 2$) cross sections (Tables II and III) differ wildly from the corresponding results of Bransden and Jundi (not given here). We have checked our calculations very carefully, and no error was found. We think that the present calculations give very reliable two-state results, although these results are not physical in the low incident energies. It can be concluded that the present method of solution is very fruitful in terms of numerical accuracy.

Figure 2 represents our results for the total elastic cross section from $k = 0.2$ to 1 (a.u.). The results of Callaway *et al.*,[17] who have used the extended polarized-orbital method, are given for comparison. They have included the effect of polarization but have neglected the effect of the rearrangement channel. On the other hand, the effect of Ps formation (virtual or real) has been taken into account in our calculation. In the framework of the close-coupling approximation, the effect of this polarization may be accounted for appreciably by including the $2p$ states of the target atom. We have neglected all the excited states of the hydrogen as well as Ps atoms in our calculations. The feature of the present curve may be changed to some extent when the polarization of both the hydrogen and Ps atoms are taken into consideration.

In Tables II and III, we have given the contribution to the total elastic cross section for each value of l. It is to be noted that our calculated value for the elastic cross section differs from the corresponding Born result even at 200 eV by about 11% (Born: 0.154; present: 0.139). A similar discrepancy with the Born results has also been noticed by Chaudhuri *et al.*[5] (Born: 0.154; Born-Oppenheimer: 0.172; and Chaudhuri *et al.*: 0.173 at 200 eV) who have investigated the e^--H scattering problem. The results for the total cross section at high energies are not expected to change appreciably if one includes the effect of polarization. The Born approximation is expected to be valid when the cross sections for both e^--H and e^+-H scattering are the same. Moreover, since the effect of polarization is attractive in nature, it will only in-

TABLE II. Total cross sections (in units of πa_0^2) for e^+-H elastic scattering below the Ps-formation threshold. The notation $a-b$ stands for $a\times10^{-b}$.

E (eV) \ l	0	1	Sum
0.1	0.8493−1	0.4358−3	0.8536−1
0.3	0.1181	0.3171−2	0.1212
0.5	0.1536	0.7106−2	0.1607
0.7	0.1904	0.1132−1	0.2017
1.0	0.2462	0.1702−1	0.2632
2.0	0.4151	0.2705−1	0.4421
3.0	0.5390	0.2829−1	0.5673
4.0	0.6175	0.2715−1	0.6446
5.0	0.6607	0.2595−1	0.6866
6.0	0.6798	0.2586−1	0.7056

crease the difference. However, it will be of great interest to observe the behavior of the total cross sections at high energies by taking into account the effects of long-range forces for both the hydrogen and Ps atoms.

Figure 3 shows our curve for the Ps-formation cross sections from the Ps-formation threshold to 50 eV. This figure also includes the works due to Mandal *et al.*[18] and Banerji *et al.*[1] for comparison. The present results differ appreciably from all other results given in the curve. The peak value obtained by us is approximately 0.6 times the Born peak. On the other hand, the position of the peak in the present approximation is around 16 eV whereas the corresponding position in Born approximation is around 13 eV. In the case of the rearrangement channel, the Born or any other similar approximation is not adequate in the low-energy region. This has been reestablished by the present method. This feature has also been noticed by Bransden and Jundi.[10]

Table IV represents the partial cross sections for Ps formation in the energy range of Ps-formation threshold to 200 eV. Two-state results for the inelastic cross sections are not at all valid in the low-energy region.[13,15] These two-state results in the low-energy region are tabulated purely from the point of academic interest. Because of the neglect of the polarization effect of the positronium atom which is eight times greater than that of the hydrogen atom, the results are expected to change appreciably. Moreover, because of short-range effects as mentioned in Refs. 13 and 15, the low-energy predicted values are subject to much change. However, nothing specific can be said about the high-energy results. The Born amplitude has also been obtained for each value of l for comparison. In the high-energy region, our calculated values also differ from the Born results appreciably.

TABLE III. Total cross sections (in units of πa_0^2) for e^+-H elastic scattering above the positronium-formation threshold. The notation $a-b$ stands for $a\times10^{-b}$.

E (eV) \ l	0	1	2	3	4	5	6	7	8	9	10	11	Sum
8.0	0.6727	0.2717−1	0.7385−1	0.1074−1	0.7640−3								0.7852
9.0	0.6681	0.2150−1	0.8809−1	0.1797−1	0.1492−2	0.9274−4							0.7973
10.0	0.6602	0.1755−1	0.9366−1	0.2347−1	0.2501−2	0.1824−3							0.7976
11.0	0.6496	0.1549−1	0.9454−1	0.2846−1	0.3641−2	0.3130−3	0.2190−4						0.7921
13.6	0.6152	0.1686−1	0.8819−1	0.3465−1	0.6340−2	0.7762−3	0.7519−4						0.7621
20.0	0.5216	0.4350−1	0.6885−1	0.3175−1	0.8653−2	0.1715−2	0.2734−3	0.3738−4					0.6764
30.0	0.3992	0.1206	0.5571−1	0.2132−1	0.6785−2	0.1799−2	0.4083−3	0.8168−4	0.1478−4				0.6059
54.4	0.2428	0.1266	0.4360−1	0.1389−1	0.4255−2	0.1249−2	0.3478−3	0.9167−4	0.2290−4	0.5439−5			0.4328
100.0	0.1233	0.7940−1	0.3353−1	0.1265−1	0.4496−2	0.1534−2	0.5065−3	0.1628−3	0.5106−4	0.1567−4			0.2556
200.0	0.5208−1	0.4198−1	0.2319−1	0.1155−1	0.5448−2	0.2475−2	0.1094−2	0.4731−3	0.2009−3	0.8408−4	0.3474−4	0.1419−4	0.1386

TABLE IV. Total cross sections (in units of πa_0^2) for the positronium formation in e^+-H collision above the threshold energy. The notation $a-b$ stands for $a\times10^{-b}$.

E (eV) \ l	0	1	2	3	4	5	6	7	8	9	10	11	Sum [c]
8.0	0.9579−4 [a]	0.2150	0.2219	0.4318−1	0.4405−2								0.4846
	0.6320 [b]	0.9120	0.3391	0.4692−1	0.4484−2								1.9346
9.0	0.2886−3 [a]	0.3071	0.4947	0.1740	0.3160−1	0.4286−2							1.0119
	0.6618 [b]	1.2117	0.8086	0.1981	0.3252−1	0.4313−2							2.9171
10.0	0.5438−3 [a]	0.3584	0.6980	0.3372	0.8543−1	0.1597−1							1.4956
	0.6362 [b]	1.2352	1.1456	0.3941	0.8895−1	0.1612−1							3.5163
11.0	0.8264−3 [a]	0.3897	0.8334	0.4851	0.1539	0.3590−1	0.7115−2						1.9060
	0.5928 [b]	1.1471	1.3250	0.5743	0.1618	0.3638−1	0.7139−2						3.8446
13.6	0.1527−2 [a]	0.4323	0.9864	0.7220	0.3196	0.1064	0.2997−1						2.5982
	0.4694 [b]	0.8153	1.3497	0.8390	0.3399	0.1087	0.3017−1						3.9521
20.0	0.2225−2 [a]	0.4865	0.8976	0.7390	0.4399	0.2125	0.8886−1	0.3358−1					2.9001
	0.2524 [b]	0.3011	0.8195	0.7444	0.4508	0.2164	0.8971−1	0.3372−1					2.9079
30.0	0.1362−3 [a]	0.4312	0.5205	0.4429	0.3062	0.1820	0.9652−1	0.4692−1	0.2133−1				2.0476
	0.1013 [b]	0.7578−1	0.3221	0.3739	0.2890	0.1790	0.9625−1	0.4696−1	0.2135−1				1.5057
54.4	0.3121−2 [a]	0.5798−1	0.9336−1	0.9590−1	0.7921−1	0.5692−1	0.3703−1	0.2235−1	0.1271−1	0.6895−2			0.4655
	0.1576−1 [b]	0.7353−2	0.4909−1	0.7215−1	0.6906−1	0.5322−1	0.3585−1	0.2201−1	0.1262−1	0.6874−2			0.3440
100.0	0.2155−3 [a]	0.5060−2	0.8970−2	0.1037−1	0.9651−2	0.7830−2	0.5768−2	0.3953−2	0.2560−2	0.1585−2	0.9459−3	0.5472−3	0.5803−1
	0.1283−2 [b]	0.6101−3	0.4610−2	0.7650−2	0.8254−2	0.7195−2	0.5503−2	0.3850−2	0.2523−2	0.1572−2	0.9416−3	0.5458−3	0.4511−1
200.0	0.5727−4 [a]	0.2889−3	0.4709−3	0.5408−3	0.5173−3	0.4400−3	0.3440−3	0.2523−3	0.1759−3	0.1177−3	0.7611−4	0.4781−4	0.3376−2
	0.4087−4 [b]	0.3197−4	0.2098−3	0.3609−3	0.4136−3	0.3863−3	0.3183−3	0.2406−3	0.1709−3	0.1156−3	0.7525−4	0.4747−4	0.2458−2

[a] Present results.

[b] Results of Banerji *et al.*, Ref. 1. (There is a slight numerical error in the previous calculation. Corrected results are given here.)

[c] Summations have been performed taking contributions of partial waves up to $l=14$ at 100 and 200 eV.

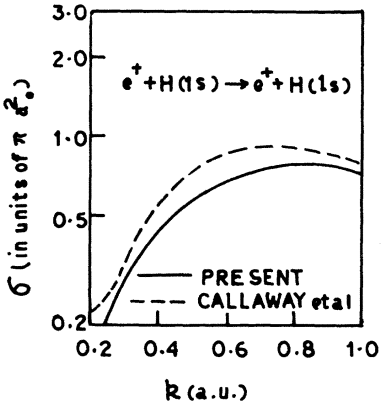

FIG. 2. Total cross sections (in units of πa_0^2) for positron-hydrogen elastic scattering as a function of k (a.u.).

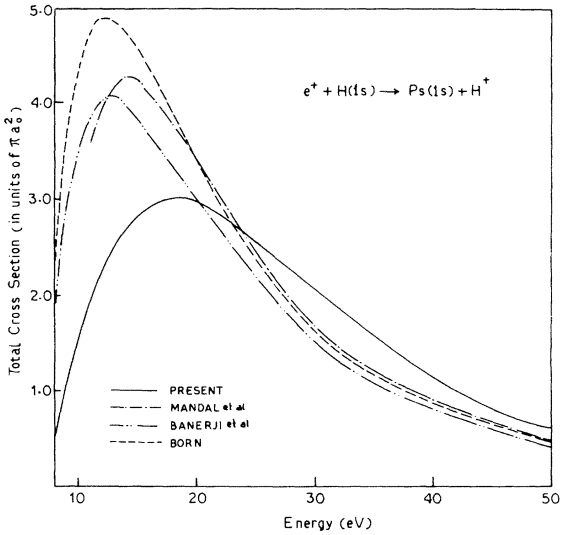

FIG. 3. Total cross sections (in units of πa_0^2) for positronium formation as a function of incident positron energy in eV.

The present results suggest that in all the energy regions, especially at high and intermediate energies, more sophisticated calculations and experimental measurements are required to ascertain the exact behavior of the cross sections.

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APPENDIX

The aim of this Appendix is to obtain the expression for $g_l^B(k_3', k_1)$. The Born amplitude $g^B(\hat{k}_3' \cdot \hat{k}_1)$ for the Ps formation has been obtained by Cheshire[19] where the on-shell relation has been used. Here we have not made use of that conservation relation. It may be written as

$$g^B(\hat{k}_3' \cdot \hat{k}_1) = -\frac{\mu_3}{2\pi}\int d\vec{r}_1\, d\vec{r}_2 \exp[-\tfrac{1}{2} i\vec{k}_3' \cdot (\vec{r}_1+\vec{r}_2)]\, \phi_{Ps}^*(|\vec{r}_1-\vec{r}_2|)\left(\frac{1}{r_1}-\frac{1}{r_2}\right)\phi_{1s}(r_2)\exp(i\vec{k}_1\cdot\vec{r}_1)$$

$$= -\frac{1}{2\sqrt{2}\,\pi^2}\int d\vec{r}_1\, d\vec{r}_2 \exp(-\tfrac{1}{2}|\vec{r}_1-\vec{r}_2| - r_2)\left(\frac{1}{r_1}-\frac{1}{r_2}\right)\exp[-\tfrac{1}{2} i\vec{k}_3'\cdot\vec{r}_2 + i(\vec{k}_1 - \tfrac{1}{2}\vec{k}_3')\cdot\vec{r}_1]. \quad \text{(A1)}$$

Using the Fourier transforms for the functions $\exp(-\frac{1}{2}|\vec{r}_1-\vec{r}_2|)$, $\exp(-\vec{r}_2)$, and $(1/r_2)\exp(-\vec{r}_2)$ and the Feynman parametrization formula,[20] the integral in (A1) may be evaluated to yield

$$g^B(\hat{k}_3' \cdot \hat{k}_1) = -\sqrt{2}\left[\int_0^1 dx \frac{x(1-x)}{\mu^5}\left(\frac{3}{\omega^2+\mu^2} + \frac{4\mu^2}{(\omega^2+\mu^2)^2} + \frac{8\mu^4}{(\omega^2+\mu^2)^3}\right) - 8\int_0^1 \frac{x\,dx}{(\omega^2+\mu^2)^3}\right], \quad \text{(A2)}$$

where

$$\mu^2 = 1 - 0.75x + 0.25x(1-x)k_3'^2 \quad \text{and} \quad \vec{\omega} = \vec{k}_1 - (1-0.5x)\vec{k}_3'.$$

We have expressed g^B [Eq. (8)] as

$$g^B(\hat{k}_3' \cdot \hat{k}_1) = \frac{1}{\sqrt{k_3'\,k_1}} \sum_{l=0}^{\infty} (2l+1) g_l^B(k_3', k_1) P_l(\hat{k}_3' \cdot \hat{k}_1). \quad \text{(A3)}$$

From (A2) and (A3) one may obtain

$$g_l^B(k_3', k_1) = -\frac{\sqrt{2}}{\pi k_3'}\left[\int_0^1 dx \frac{x(1-x)}{\mu^5(2-x)}\left(3Q_l(t) - \frac{4\mu^2 Q_l'(t)}{k_3' k_1(2-x)} + \frac{4\mu^4 Q_l''(t)}{k_3'^2 k_1^2(2-x)^2}\right) - \frac{4}{k_3'^2 k_1^2}\int_0^1 \frac{x Q_l''(t)}{(2-x)^3}\,dx\right], \quad \text{(A4)}$$

where

$$t = \frac{(4k_1^2 + k_3'^2 + 1)}{4k_1 k_3'}.$$

The resulting one-dimensional integration has been performed numerically. The overlap integral coming from the off-shell amplitude may be evaluated in the same fashion.

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