Positron-hydrogen collisions at low energies

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The Harris-Nesbet algebraic method was used to carry out a large coupled-state calculation of e^+-H scattering at energies below the first excitation threshold of hydrogen. The six-state ($1s,2s,2p$ H–$1s,2s,2p$ Ps) coupling scheme was extended to include an adequate number of short-ranged functions of both hydrogenic and positroniumic types and the H $3\overline{p}$ pseudostate. Phase shifts and cross sections of partial waves from $L=0$ to 6 were obtained for e^+-H ($1s$) scattering as well as for Ps($1s$)-p scattering. Our results are to be compared with those obtained by other research groups with some large-scale calculations employing, however, different numerical methods of approach. Our results agree excellently with the values calculated with a variational method by Bhatia *et al.* and by Humberston and co-workers and with the 21-state close-coupling approximation by Mitroy and co-workers. [S1050-2947(96)02512-7]

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INTRODUCTION

There has been a surge of theoretical research interest recently in positron scattering from atomic hydrogen. This is probably due in part to the fact that experimental data of total cross section and positronium-formation cross section for e^+-H collisions have been made available in the literature of the recent years [1,2]. Phase shifts and cross sections for e^+-H scattering at energies below the first excitation threshold of H had already been carried out one or two decades ago by Bhatia *et al.* [3] and by Humberston and co-workers [4] with a variational method. However, these authors limited their calculations to only a few lowest (S, P, and D) partial waves. In order to obtain the positronium-formation and total cross sections for comparison with experimental data, various theoretical groups [5–7] recently resorted to the close-coupling (coupled-state) approximation, in which the size of the coupling scheme was gradually increased to adequately accommodate the various scattering effects. Within the close-coupling (coupled-state) approximation, cross sections could be obtained for higher partial waves and total cross sections could then be deduced. These research groups employed either the R-matrix method [5,6] or the method of solving the coupled Lippmann-Schwinger equations in momentum space [7]. To our knowledge, the largest coupling scheme that the first group [6] used for their (published) calculation was an 18-state one, while that of the second [7] was a 21-state one. The results of both groups for low partial waves agree well with those obtained with the variational method [3,4].

For some time [8–11], the Harris-Nesbet method has been used also to carry out coupled-state (close-coupling) calculations for positron-hydrogen scattering. This algebraic method of approach had been developed earlier by Harris [12] and Nesbet [13] and had been considered by Seiler, Obero, and Callaway [14] and by Wakid and Labahn [15] for positron scattering. Wakid and Labahn [15], however, had carried out the calculation for S-wave scattering and small coupling schemes only. Earlier works [8–11] indicated that the method can handle the positronium formation channel well. It can also provide numerically accurate results of cross section especially at low energies. Because of its high numerical accuracy, the method has also been used to successfully investigate other relevant interesting problems of e^+-H collision, such as Feshbach resonances [10] and resonances at medium energy [11]. Earlier works [9,10] also demonstrated that the method is quite feasible for high partial wave ($L \geqslant 6$) e^+-H scattering and for any large coupling scheme and that an extension of the calculation to any large scheme could be achieved without any difficulty. This paper reports the results of such a large calculation. The purpose of this calculation is to obtain, with the Harris-Nesbet method, the so-called ''accurate'' values of cross section at low energies. These results are to be compared with those obtained with other methods of approximation, especially with the ones calculated with a variational method [3,4] and with the 21-state close-coupling approximation [7].

I. METHOD

The two methods that have been used to obtain accurate phase shifts and cross sections in coupled-state (close-coupling) calculations have been well known. One is the use of a large set of H and Ps pseudostates to simulate the physical bound states and continuum of the collision system. Another is the use of a large set of short-range L^2 (or correlation) functions for this simulation. Both methods can be traced to early works by various authors some 30 years ago [16–18]. Register and Poe [19] had carried out a large Harris-Nesbet calculation with the use of Hylleraas-type correlation functions. However, these authors limited their calculation to S, P, and D partial waves only and did not seem to consider the Ps-formation channels in their calculation.

Thus in this work, a Harris-Nesbet calculation has been carried out with its coupling scheme extended from the six-state one [9] to include short-range functions (through the correlation terms) and the pseudostate H $3\overline{p}$. Following Chan and co-workers [20], the Slater-type short-range functions have been chosen for the calculation. Both the hydrogenic

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TABLE I. S- and P-wave shifts (in radians) for positron-hydrogen scattering at energies below the positronium-formation threshold. The numbers in square brackets represent powers of 10.

k (a.u.)	0.1	0.2	0.3	0.4	0.5	0.6	0.7
			$L=0$				
Present Harris-Nesbet	0.1483	0.1875	0.1670	0.1195	0.620[−1]	0.330[−2]	−0.519[−1]
Variational[a]	0.1483	0.1877	0.1677	0.1201	0.624[−1]	0.39[−2]	−0.512[−1]
21-state[b]	0.1474	0.1868	0.1667	0.1191	0.621[−1]	0.31[−2]	−0.518[−1]
Harris-Nesbet[c]	0.1460	0.1849	0.1649	0.1172	0.593[−1]	−0.3[−4]	−0.569[−1]
Schwinger[d]	0.1473	0.1869	0.1671	0.1202	0.631[−1]	0.41[−2]	−0.514[−1]
IERM[e]	0.148	0.187	0.167	0.118	0.62[−1]	0.4[−2]	
Faddeev[f]	0.149	0.189	0.169	0.121	0.62[−1]	0.3[−2]	−0.50[−1]
			$L=1$				
Present Harris-Nesbet	0.886[−2]	0.327[−1]	0.657[−1]	0.1002	0.1305	0.1544	0.1782
Variational[a]		0.338[−1]	0.665[−1]	0.1016	0.1309	0.1547	0.1799
21-state[b]	0.887[−2]	0.327[−1]	0.657[−1]	0.1002	0.1306	0.1542	0.1788
Harris-Nesbet[c]	0.5[−2]	0.30[−1]	0.63[−1]	0.97[−1]	0.128	0.146	0.169
Schwinger[d]	0.88[−2]	0.333[−1]	0.658[−1]	0.1012	0.1318	0.1534	0.1739
IERM[e]	0.9[−2]	0.33[−1]	0.66[−1]	0.102	0.132	0.156	0.185

[a]Variational calculation, Bhatia *et al.* [3].
[b]21-state close-coupling, Mitroy [7].
[c]Harris-Nesbet with correlation functions, Register and Poe [19].
[d]Schwinger-variational principle, Roy and Mandal [23].
[e]Intermediate energy R-Matrix with extrapolation, Higgins, Burke, and Walters [22].
[f]Solving the modified Faddeev equations, Kvitsinsky and co-workers [25].

and positroniumic forms were used for the short-range functions. The angular momentum of the short-range functions of the correlation terms that served to simulate other physical states of either H or Ps was limited to $l \leqslant 2$, since short-range functions of higher angular momentum are expected not to contribute to the results at low energy significantly. The total number of the correlation terms in this calculation was 126, 210, and 252 for $L=0$, $L=1$, and $L \geqslant 2$, respectively. We also added the H $3\overline{p}$ pseudostate [21] to the coupling scheme so that, together with the H $2p$ state, they can by themselves account for almost 100% of the dipole polarizability of H($1s$). For the physical channels $1s,2s,2p$ H and $1s,2s,2p$ Ps, the short-range basis functions were, as usual, chosen to be of a Slater-type $r^p e^{-Z_j r}$. In this calculation, p (an integer) was not restricted to be equal to the angular momentum l_i of the projectile of the channel only. Rather, we chose $p=l_i+n_p$ where $n_p=0$, 1, and 2. With this choice, we could obtain a good accuracy for the results of calculation with less than 18 basis functions, and with Z_j restricted to only a few not-too-small values.

The details of the formalism and numerical procedure of the Harris-Nesbet method have been described elsewhere [9,10]. It should be mentioned that a similar enlarged coupling scheme (without inclusion of the H $3\overline{p}$) was used in a calculation [10] that determined the sequences of Feshbach resonances below the $n=2$ H threshold. The numerical calculations of the Harris-Nesbet method with large coupling schemes were, indeed, found [9,10] to be easily extendible from the basic six-state one with some appropriate minor modifications.

II. RESULTS AND DISCUSSION

In Table I and II we show the results of phase shift that we calculated with this coupling scheme. In Tables III, IV, and V we present, respectively, samples of the results of elastic e^+-H, positronium formation, and elastic Ps($1s$)-p cross sections at energies in the Ore gap for comparison with those obtained by others with other methods of approximation. Table VI exhibits some values of the S-wave reactance matrix elements for comparison with values calculated by others. In Figs. 1, 2, and 3, we plot the partial wave cross sections, respectively, for Ps formation, elastic e^+-H scattering, and Ps($1s$)-p elastic scattering. In Fig. 4 we show our results of Ps-formation, integrated elastic, and total cross sections. In Fig. 5 we plot our H-formation cross sections and in Fig. 6 our integrated Ps-p elastic, total H-formation, and total cross sections for Ps($1s$)-p scattering.

Our results of phase shift (see Table 1) agree excellently with those calculated with the variational method [3] for S- and P-wave scattering. They also agree excellently with the phase shifts (see Tables I and II) calculated with the close-coupling approximation employing a large (21-state) coupling scheme composed of pseudostates [7]. It may be worth noting that while the coupling schemes of both models (Harris-Nesbet and 21-state close coupling) were based on the six-state one, we used the short-range functions plus the H $3\overline{p}$ pseudostate to represent effects of other closed physical bound states and continuum, while Mitroy employed an additional 15 (pseudo)states for this purpose. The excellent agreement between the two sets of values seemed to confirm

TABLE II. $L=2$, 3, 4, 5, and 6 phase shifts (in radians) for positron-hydrogen scattering. The numbers in square brackets indicate powers of 10.

k (a.u.)	0.1	0.2	0.3	0.4	0.5	0.6	0.7
			$L=2$				
Present Harris-Nesbet	0.133[−2]	0.549[−2]	0.129[−1]	0.241[−1]	0.396[−1]	0.597[−1]	0.883[−1]
21-state[a]	0.136[−2]	0.551[−2]	0.129[−1]	0.242[−1]	0.397[−1]	0.598[−1]	0.885[−1]
Harris-Nesbet[b]	0.13[−2]	0.54[−2]	0.125[−1]	0.235[−1]	0.389[−1]	0.593[−1]	0.863[−1]
Schwinger[c]	0.131[−2]	0.543[−2]	0.126[−1]	0.2348[−1]	0.3817[−1]	0.5925[−1]	0.8697[−1]
IERM[d]		0.5[−2]	0.13[−1]	0.25[−1]	0.41[−1]	0.62[−1]	
			$L=3$				
Present Harris-Nesbet	0.435[−3]	0.177[−2]	0.406[−2]	0.750[−2]	0.125[−1]	0.197[−1]	0.305[−1]
21-state[a]	0.452[−3]	0.180[−2]	0.409[−2]	0.754[−2]	0.126[−1]	0.198[−1]	0.307[−1]
Schwinger[c]	0.454[−3]	0.178[−2]	0.404[−2]	0.710[−2]	0.133[−1]	0.161[−1]	0.218[−1]
IERM[d]		0.18[−]	0.4[−2]	0.75[−2]	0.126[−1]	0.207[−1]	
			$L=4$				
Present Harris-Nesbet	0.193[−3]	0.793[−3]	0.180[−2]	0.325[−2]	0.525[−2]	0.799[−2]	0.119[−1]
21-state[a]	0.205[−3]	0.819[−3]	0.183[−2]	0.329[−2]	0.530[−2]	0.807[−2]	0.121[−1]
Schwinger[c]	0.204[−3]	0.813[−3]	0.188[−2]	0.323[−2]	0.507[−2]	0.746[−2]	0.994[−2]
			$L=5$				
Present Harris-Nesbet	0.100[−3]	0.420[−3]	0.958[−3]	0.172[−2]	0.272[−2]	0.403[−2]	0.576[−2]
21-state[a]	0.109[−3]	0.443[−3]	0.986[−3]	0.175[−2]	0.277[−2]	0.410[−2]	0.587[−2]
Schwinger[c]	0.109[−3]	0.436[−3]	0.987[−3]	0.177[−2]	0.273[−2]	0.396[−2]	0.535[−2]
			$L=6$				
Present Harris-Nesbet	0.571[−4]	0.248[−3]	0.566[−3]	0.101[−2]	0.160[−2]	0.234[−2]	0.327[−2]
21-state[a]	0.633[−4]	0.266[−3]	0.593[−3]	0.105[−2]	0.165[−2]	0.241[−2]	0.336[−2]
Schwinger[c]	0.650[−4]	0.259[−3]	0.589[−3]	0.105[−2]	0.167[−2]	0.234[−2]	0.326[−2]
			σ_{elastic}				
Present Harris-Nesbet	8.828	3.815	1.848	1.194	1.025	1.029	1.181
21-state[a]	8.736	3.787	1.844	1.192	1.026	1.026	1.186

[a]21-state close-coupling, Mitroy [7].

[b]Harris-Nesbet with correlation functions, Register and Poe [19].

[c]Schwinger principle, Roy and Mandal [23].

[d]Intermediate energy R-matrix with extrapolation, Higgins, Burke, and Walters [22].

an equivalence between the use of either (pseudo)states or short-range functions. The S- and P-wave phase shifts calculated by Register and Poe [19] with the Harris-Nesbet method are about 2–10% smaller than ours. This may be because the number of (Hylleraas-type) correlation functions (84) that they incorporated in their calculation was smaller. The S- and P-wave phase shifts calculated with the intermediate energy R-matrix (IERM) [22] method are also in good agreement with ours (see Table I). So are those obtained by Roy and Mandal [23] with the Schwinger-variational method. The D-wave phase shifts calculated by Register and Poe [19] are about 2% smaller than ours. The D-wave phase shifts obtained with the Schwinger-variational method [23] for $k \leqslant 0.4a_0^{-1}$ agree well with ours but they are slightly smaller than ours by about 2% at higher energies. The IERM values of the D-wave phase shifts [22] are only in fair agreement with ours (see Table II).

For higher partial waves ($L=3$, 4, 5, and 6) our phase shifts still agree very well (see Table II) with the ones obtained with the 21-state close-coupling calculation [7], except for values at momentum $k=0.1a_0^{-1}$, $0.2a_0^{-1}$, and $0.3a_0^{-1}$. The cause for this slight discrepancy is not clear. The slight discrepancy might be due to the fact that our coupling scheme may not represent well the long-range effect of the continuum wave functions at low energy and high angular momentum where this effect becomes important. It may also be due, in part, to the numerical uncertainty that does exist in these numerical methods, especially at low energy and high angular momentum. However, the contribution to the total elastic cross sections from $L \geqslant 3$ partial wave scattering is very small at low energies to make this discrepancy worth any concern.

We also tentatively calculated S-wave phase shifts at positron momentum values down to about $k=0.001a_0^{-1}$ and then deduced, by a direct extrapolation of $k\cot(\delta_s)$ to $k=0$, a scattering length of $A_0=-2.101a_0$. This value of scattering length agrees very well with the variational values of Houston and Drachman [24] $[(-2.1036\pm0.0004)a_0]$ and by Humberston and co-workers [4] $[(-2.103\pm0.001)a_0]$. It also agrees well with the value $[(2.104\pm0.001)a_0]$ obtained by the method of solving the Faddeev equations [23], and with the value obtained by a 21-state close-coupling calculation [7] $[(-2.08\pm0.02)a_0]$.

The integrated elastic cross sections shown in Table II

TABLE III. Partial wave elastic cross sections (in units of πa_0^2) for positron-hydrogen scattering at energies in the Ore gap. The numbers in square brackets indicate powers of 10.

k (a.u.)	0.71	0.75	0.80	0.85
		$L=0$		
Present Harris-Nesbet	0.258[−1]	0.431[−1]	0.652[−1]	0.859[−1]
Variational[a]	0.26[−1]	0.43[−1]	0.65[−1]	0.85[−1]
21-state[b]	0.258[−1]	0.430[−1]	0.657[−1]	0.849[−1]
Hyperspherical[c]	0.33[−1]	0.50[−1]	0.76[−1]	0.100
Hyperspherical[d]	0.325[−1]	0.548[−1]	0.838[−1]	0.111
Hyperspherical[e]	0.234[−1]	0.415[−1]	0.637[−1]	0.863[−1]
Faddeev[f]	0.25[−1]	0.44[−1]	0.63[−1]	
		$L=1$		
Present Harris-Nesbet	0.800	0.723	0.624	0.549
Variational[a]	0.789	0.724	0.622	0.547
21-state[b]	0.802	0.726	0.626	0.551
Hyperspherical[d]	0.748	0.650	0.532	0.449
Hyperspherical[e]	0.810	0.720	0.608	0.528
		$L=2$		
Present Harris-Nesbet	0.339	0.444	0.482	0.474
Variational[a]	0.323	0.403	0.423	0.413
21-state[b]	0.341	0.446	0.484	0.477
Hyperspherical[d]	0.304	0.376	0.389	0.366
Hyperspherical[e]	0.330	0.401	0.420	0.391
		$L=3$		
Present Harris-Nesbet	0.568[−1]	0.773[−1]	0.110	0.134
21-state[b]	0.575[−1]	0.781[−1]	0.111	0.135
Hyperspherical[d]	0.471[−1]	0.541[−1]	0.675[−1]	0.761[−1]
Hyperspherical[e]	0.676[−1]	0.739[−1]	0.853[−1]	0.950[−1]
		Total		
Present Harris-Nesbet	1.236	1.306	1.308	1.278
21-state[b]	1.242	1.313	1.316	1.285

[a]Variational calculation, Humberston [4], Brown and Humberston [4].
[b]21-state close-coupling, Mitroy [7].
[c]Close coupling using hyperspherical-coordinate method, Archer, Parker, and Pack [26].
[d]Close coupling using hyperspherical-coordinate method, Igarashi and Toshima [27].
[e]Close coupling using hyperspherical-coordinate method, Zhou and Lin [28].
[f]Modified Faddeev-equation method, Kvitsinsky and co-workers [25].

were obtained by summing the seven lowest partial wave cross sections ($L=0,1,2,3,4,5,6$). As was expected, the agreement of these numbers with those of the 21-state close-coupling calculation [7] is very good, except for a slight discrepancy detected at positron momenta $k=0.1a_0^{-1}$ and $0.7a_0^{-1}$ (see Table II). It should also be noted that the total elastic cross sections of the 21-state calculation that we quoted were those derived by Mitroy with his 21-state phase shifts (not those obtained by him with a ''mixed'' model [7]).

We found that (see Table III) the P, D, and F partial wave cross sections contributed about 90% to the integrated elastic cross sections in the Ore gap. Our partial elastic cross sections in the Ore gap agree excellently with those calculated with the 21-state close-coupling approximation [7]. The maximum difference between the two sets of values is less than 1%. Our S- and P-wave elastic cross sections also agree excellently with those calculated with the Kohn-variational method by Humberston and co-workers [4]. However, our D-wave values are about 10–15% larger than theirs. Kernoghan and co-workers [6] also observed this significant difference through their 18-state coupled-state results that were obtained with the R-matrix method. The S- and P-wave cross sections by Archer, Parker, and Pack [26] and by Igarashi and Toshima [27], calculated with the hyperspherical-coordinate method, differ from ours by about 20%. However, those calculated by Zhou and Lin [28] with the same method are closer to ours. For D- and F-wave scattering, the cross sections calculated with this method by both groups are in general smaller than ours, especially at the high end of the Ore gap. Our S-wave values also reasonably agree with those calculated with the Faddeev equation [25]. Our present Harris-Nesbet integrated elastic cross sections in the Ore gap agree excellently with those calculated by the 21-state close-coupling approximation [7] within 1%.

Our positronium-formation cross sections in the Ore gap

TABLE IV. Partial wave Ps-formation cross sections (in units of πa_0^2) for positron-hydrogen scattering at energies in the Ore gap. The numbers in square brackets indicate powers of 10.

k (a.u.)	0.71	0.75	0.80	0.85
		$L=0$		
Present Harris-Nesbet	0.404[−2]	0.441[−2]	0.493[−2]	0.549[−2]
Variational[a]	0.41[−2]	0.44[−2]	0.49[−2]	0.58[−2]
21-state[b]	0.405[−2]	0.427[−2]	0.472[−2]	0.560[−2]
Hyperspherical[c]	0.34[−2]	0.38[−2]	0.43[−2]	0.49[−2]
Hyperspherical[d]	0.404[−2]	0.398[−2]	0.462[−2]	0.535[−2]
Hyperspherical[e]	0.407[−2]	0.421[−2]	0.473[−2]	0.553[−2]
Faddeev[f]	0.38[−2]	0.43[−2]	0.47[−2]	
		$L=1$		
Present Harris-Nesbet	0.267[−1]	0.367	0.483	0.565
Variational[a]	0.27[−1]	0.365	0.482	0.561
21-state[b]	0.266[−1]	0.366	0.483	0.563
Hyperspherical[d]	0.366[−1]	0.376	0.490	0.570
Hyperspherical[e]	0.23[−1]	0.370	0.480	0.552
		$L=2$		
Present Harris-Nesbet	0.683[−3]	0.320	0.862	1.162
Variational[a]	0.62[−3]	0.335	0.812	1.057
21-state[b]	0.682[−3]	0.320	0.859	1.158
Hyperspherical[d]	0.934[−3]	0.334	0.866	1.16
Hyperspherical[e]	0.345[−3]	0.254	0.770	1.031
		$L=3$		
Present Harris-Nesbet	0.500[−5]	0.354[−1]	0.271	0.596
21-state[b]	0.44[−5]	0.356[−1]	0.270	0.596
Hyperspherical[d]	0.573[−5]	0.382[−1]	0.276	0.592
Hyperspherical[e]	0.363[−4]	0.133[−1]	0.188	0.484
		Total		
Present Harris-Nesbet	0.315[−1]	0.729	1.666	2.499
21-state[b]	0.313[−1]	0.728	1.660	2.49

[a]Variational calculation, Humberston [4], Brown and Humberston [4].
[b]21-state close-coupling, Mitroy [7].
[c]Close coupling using hyperspherical-coordinate method, Archer, Parker, and Pack [26].
[d]Close coupling using hyperspherical-coordinate method, Igarashi and Toshima [27].
[e]Close coupling using hyperspherical-coordinate method, Zhou and Lin [28].
[f]Modified Faddeev-equation method, Kvitsinsky and co-workers [25].

(see Table IV) agree excellently with those calculated with the variational method [4] for S- and P-wave scattering. Our Ps-formation cross sections also agree excellently with those of the 21-state coupled-state method [7]. The maximum difference between the results of the two calculations is less than $0.004\pi a_0^2$. The relative difference is less than 1%, except for energies close to the Ps-formation threshold. The Ps-formation cross sections are, however, very small at these energies. In general, the D-wave variational Ps-formation cross sections by Humberston and co-workers [4] are smaller than ours by about 10%, except that at $k=0.075a_0^{-1}$, the variational value is, on the contrary, greater than ours by about 5%. The Ps-formation cross sections calculated with the hyperspherical-coordinate method by Archer *et al.* [26] are somewhat smaller than ours. However, values calculated with the same method by Igarashi and Toshima [27] and by Zhou and Lin [28] are closer to ours. The S-wave Ps-formation cross sections obtained with the Faddeev-equation method [25] also agree reasonably well with our values. The P- and D-wave hyperspherical-coordinate values of Igarashi and Toshima [27] agree well with our results except at $k=0.71a_0^{-1}$ where the relative difference is quite large. The P-wave values by Zhou and Lin, who used the same hyperspherical-coordinate method, are closer to ours, while their D-wave values are much smaller than ours. For the F wave, the cross sections by Igarashi and Toshima, on the contrary, agree well with our values, while those of Zhou and Lin are, in general, smaller.

Again, we found that the contribution from the S-wave partial cross sections to the total Ps-formation cross sections are minimal. It decreases from about 10% at $k=0.71a_0^{-1}$ to about 0.2% at $k=0.86a_0^{-1}$. The main contributors are still the P-, D-, and F-wave partial cross sections. The total Ps-formation cross sections shown were obtained by summing the partial cross sections from $L=0$ to 6. Our total Ps-formation cross sections agree very well with those of the

TABLE V. Ps-p elastic cross sections in πa_0^2 units.

Ps energy (Ry)	0.0041	0.0625	0.1400	0.2225
	$L=0$			
Present Harris-Nesbet	58.39	7.052	9.930	8.366
Variational[a]	56.7	7.05	9.93	8.37
21-state[b]	59.7	6.92	9.86	8.32
	$L=1$			
Present Harris-Nesbet	14.38	3.928	0.197	1.921
21-state[b]	15.2	4.17	0.160	1.77
	$L=2$			
Present Harris-Nesbet	0.6227	6.748	4.050	1.646
21-state[b]	0.792	7.07	4.26	1.82
	$L=3$			
Present Harris-Nesbet	0.750[−1]	1.70	3.13	3.39
21-state[b]	0.119	1.85	3.32	3.64
	Total			
Present Harris-Nesbet	73.49	20.04	18.79	17.80
21-state[b]	75.9	20.8	19.5	18.6

[a]Variational calculation, Humberston and co-workers [4].
[b]21-state close-coupling, Mitroy [7].

21-state close-coupling calculation (see Table IV). The difference is less than 1%.

We found that (see Table V) our S-wave cross sections for Ps($1s$) elastically scattered from proton agree very well with those calculated with the Kohn-variational method by Humberston [4]. Our S-wave Harris-Nesbet values were, in general, slightly greater than those calculated by Mitroy [7] with a 21-state coupling scheme. The agreement between our Harris-Nesbet P-, D-, and F-wave cross sections with those of the 21-state coupled-state calculation is only fair. The discrepancy between the two sets of cross sections was found,

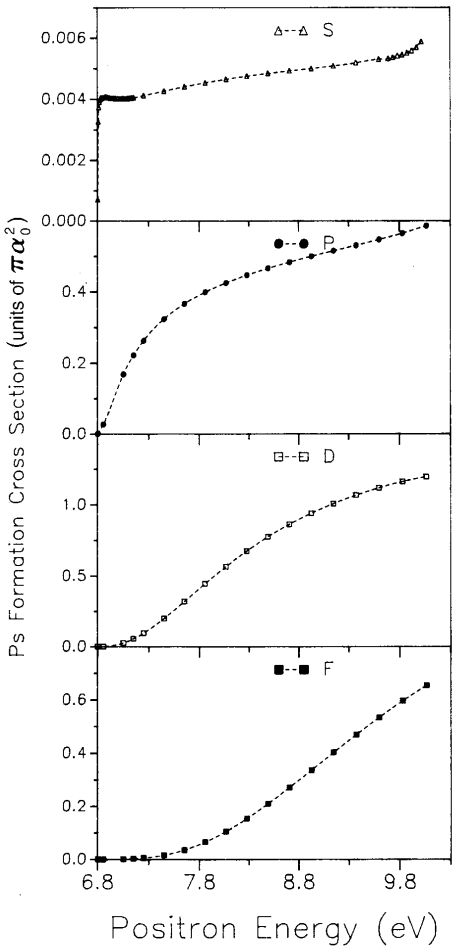

FIG. 1. Ps-formation cross sections in units of πa_0^2 at energies in the Ore gap. ○---○: P wave; □---□: D wave; ■---■: F wave; △---△: S wave.

TABLE VI. Comparison of the S-wave reactance matrices obtained by different methods. The numbers in square brackets indicate powers of 10.

k (a.u.)	Type	R_{11}	R_{12}	R_{22}
0.71	Present Harris-Nesbet	−0.5695[−1]	−0.2411[−1]	0.3689
	Variational[a]	−0.57[−1]	−0.24[−1]	0.363
	Faddeev[b]	−0.565[−1]	−0.232[−1]	0.348
	Faddeev[c]	−0.59[−1]	−0.24[−1]	0.33
0.75	Present Harris-Nesbet	−0.7850[−1]	−0.2831[−1]	−0.5321
	Variational[a]	−0.78[−1]	−0.28[−1]	−0.532
	Faddeev[b]	−0.793[−1]	−0.280[−1]	−0.536
	Faddeev[c]	−0.85[−1]	−0.29[−1]	−0.54
0.80	Present Harris-Nesbet	−0.1040	−0.5125[−1]	−1.514
	Variational[a]	−0.104	−0.51[−1]	−1.513
	Faddeev[b]	−0.102	−0.50[−1]	−1.512
	Faddeev[c]	−0.109	−0.52[−1]	−1.52
0.85	Present Harris-Nesbet	−0.1294	−0.1224	−3.722
	Variational[a]	−0.130	−0.126	−3.735
	Faddeev[c]	−0.169	−0.425	−6.40

[a]Variational method, Humberston [4].
[b]Modified Faddeev-equation method, Kvitsinsky and co-workers [25].
[c]Faddeev-equation method, Kvitsinsky and co-workers [25].

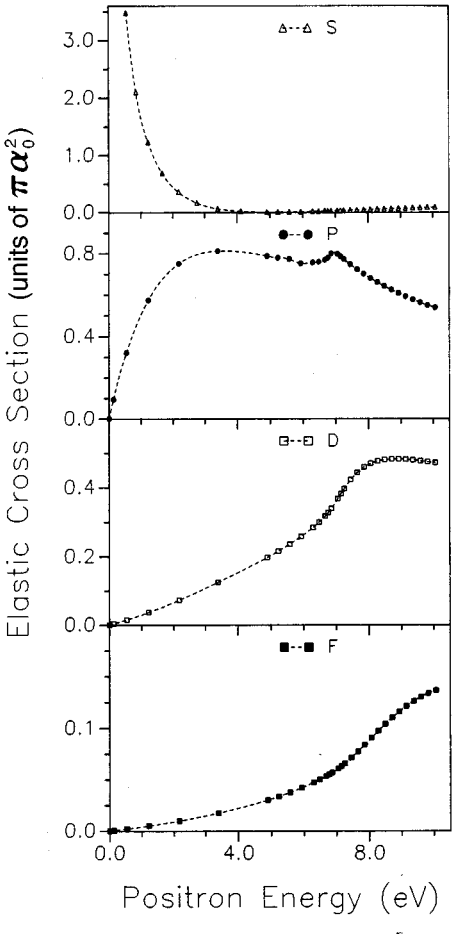

FIG. 2. e^+-H elastic scattering cross sections in units of πa_0^2 at energies below the first excitation threshold of hydrogen. Same as in Fig. 1.

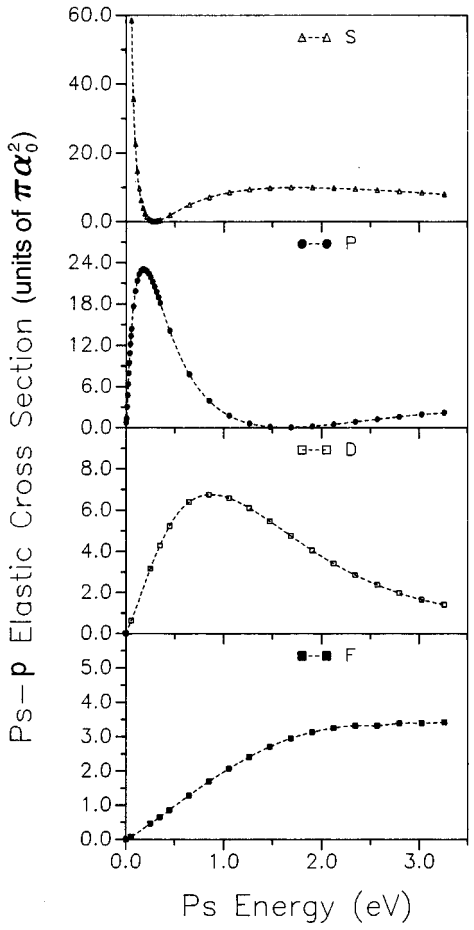

FIG. 3. Ps($1s$)-p elastic scattering cross sections in units of πa_0^2 at positron energies in the Ore gap. Same as in Fig. 1.

however, not to exceed 10%, except at very low energies where the discrepancy becomes greater (see Table V). An incomplete account of our coupling scheme for 100% of the dipole polarizability of Ps($1s$) should be responsible for it. The numerical uncertainty of the numerical methods might also, in part, be the source for this discrepancy. Our total Ps($1s$)-p elastic cross sections only agree fairly with those of Mitroy (see Table V). The two sets of values differ from each other by about 5%.

By diagonalizing the reactance matrix, we calculated the S-wave eigenphase shifts of elastic Ps scattering down to $k_p = 0.017\,895\,72 a_0^{-1}$ and then by a direct extrapolation of $k_p \cot(\delta_S)$ to $k_p = 0$, we deduced a scattering length of $A_0 = -14.48 a_0$ for the p-Ps($1s$) elastic cross section. This value is to be compared with $(-15.1 \pm 0.2) a_0$ which was the one obtained by Mitroy [7] in his 21-state close-coupling calculation. The threshold cross section for Ps($1s$)-p scattering of our calculation is, therefore, about $840 \pi a_0^2$.

Our S-wave matrix elements of the reactance matrix (see Table VI) agree very well with those calculated with the variational method [4]. The agreement between our values and those obtained with the Faddeev-equation method [25] is somewhat worse.

Our total cross sections (sum of the integrated elastic and Ps-formation cross sections) agree fairly (in the sense of Fig. 4) with experimental data of Zhou *et al.* [1]. Regarding their experiment, it may be worth noting that there has been some difficulty with the discrimination against incident positrons going into small scattering angles, and this difficulty may somewhat distort its results of cross section. Our

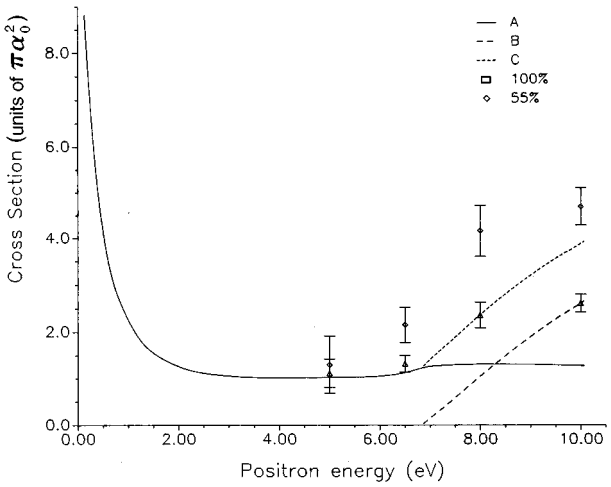

FIG. 4. Integrated elastic, total Ps formation, and total cross sections in πa_0^2 units. Curve A: integrated elastic; curve B: Ps formation; curve C: total; ⟠: experimental data, Zhou *et al.* 55% [1]; ⟠: Experimental data, Zhou *et al.* 100% [1].

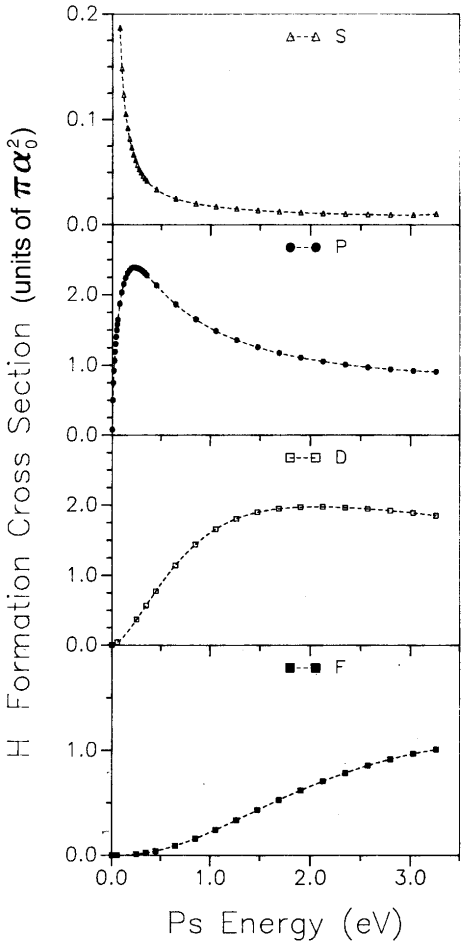

FIG. 5. H-formation cross sections in units of πa_0^2 at positron energies in the Ore gap. Same as in Fig. 1.

H-formation cross sections shown in Figs. 5 and 6 agree reasonably well with those calculated with the 21-state close-coupling approximation [7]. It should also be noted that if CP invariance is respected, the H-formation cross sections also represent the antihydrogen formation cross sections in Ps$(1s)$-$\bar{p}$ collisions at low energies.

CONCLUSION

In this paper we reported the results of a Harris-Nesbet calculation of e^+-H scattering at low energies, using a large coupling scheme that was extended from the six-state one to include an adequate number of short-range functions *and* the H $3\bar{p}$ pseudostate. The purpose of this calculation is to obtain accurate coupled-state phase shifts and cross sections at low energies with the Harris-Nesbet algebraic method. At positron energies below the $n=2$ H excitation threshold, our Harris-Nesbet results of phase shift, elastic, and Ps-formation cross sections calculated with this coupling scheme for the e^+-H entrance channel agree very well with those calculated with a variational method [3,4] and excellently with those of the 21-state close-coupling (coupled-state) approximation, using large coupling schemes composed of pseudostates [7]. This good agreement seemed to confirm an equivalence between the two approaches (pseudostates and short-range or correlation functions) for coupled-state (close-coupling) calculations at low energies. However, our cross sections for Ps$(1s)$-p scattering only agree fairly with those of the 21-state close-coupling approximation. To complement the present work, we have also been carrying out a Harris-Nesbet calculation of e^+-H collisions at low energies, employing large coupling schemes composed, however, of pseudostates (18 and 20 states). Since these coupling schemes contain the degenerate $2s$ and $2p$ H states, we may, as well, tentatively repeat a similar hunt, with these coupling schemes, for the sequences of S, P, and D resonances that, within work [10] on the theory of Feshbach resonance in e^+-H scattering, were previously found below the $n=2$ H threshold.

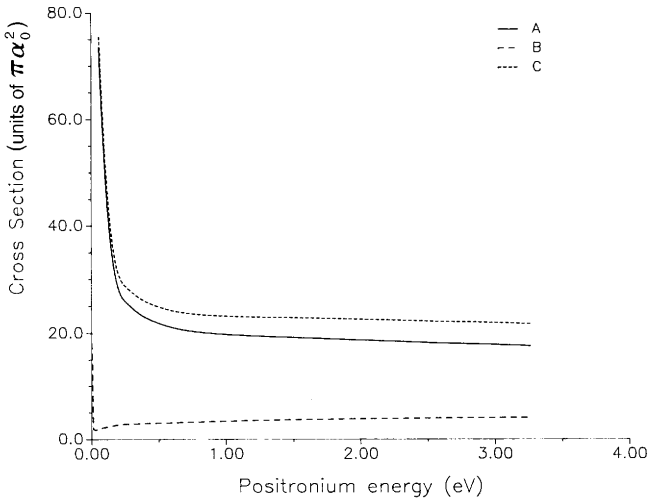

FIG. 6. Integrated elastic, total H formation, and total cross sections for Ps$(1s)$-p scatterings in πa_0^2 units. Curve A: integrated elastic; curve B: H formation; curve C: total.

Note added in proof. A recent calculation by one of us (T.T.G.), with the Ps $3\bar{p}$ pseudostate added to this coupling scheme, provided accurate results for Ps $(1s)$-p cross sections as well. Theoretical data of the calculation with this further enlarged scheme will be supplied on request for comparison.

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