# Coupled-state calculations of positron-hydrogen scattering

T. T. Gien

Department of Physics, Memorial University of Newfoundland, St. John's, Newfoundland, Canada A1B 3X7 (Received 25 November 1996; revised manuscript received 31 March 1997)

An algebraic coupled-state calculation of positron-hydrogen scattering carried out with an enlarged eightstate (E8S) coupling scheme, that is composed of a sufficiently high number of short-ranged correlation terms and eight hydrogen and positronium states [(1s,2s,2p,3p)H-(1s,2s,2p,3p)Ps], provides results of the phase shift and cross section, agreeing excellently with our accurate enlarged six pseudostate (E6PS) values in both  $e^+$ -H and Ps(1s)-p entrance channels. Our results serve to assert that very accurate values of the phase shift and cross section in both entrance channels have been attained with our E6PS, E8PS, and E8S Harris-Nesbet calculations. The present E8S calculation supersedes our deficient modified enlarged six-state one done previously. [S1050-2947(97)02708-X]

PACS number(s): 34.90.+q

## INTRODUCTION

We have recently [1-3] carried out Harris-Nesbet [4] calculations for  $e^+$ -H scattering with large coupling schemes using correlation functions. To obtain "accurate" scattering phase shifts and cross sections at positron energies below the n=2 H threshold, we used the so-called enlarged sixpseudostate (E6PS) scheme [2] for the calculation. This enlarged scheme was built with a sufficiently high number of correlation terms on the six pseudostate  $[(1s,2\overline{s},2\overline{p})H - (1s,2\overline{s},2\overline{p})Ps]$  one [5,6]. The E6PS calculation, indeed, produced (by a single calculation) the most accurate results of phase shift and cross section for both  $e^+$ -H and Ps(1s)-p entrance channels [2].

In another (alternative) calculation (which was designed for a possible extension to higher energies) [3], we instead chose the large scheme [the so-called enlarged six-state (E6S) one] that had been used [1] in a calculation which redetermined the sequences of Feshbach resonances found beneath the n = 2 H threshold previously [7] and added to it the H  $3\overline{p}$  pseudostate [8] to (partially) repair the deficiency of the "polarization" of the scheme. This so-called modified enlarged six-state scheme (ME6S) [2,3], while being more cumbersome than the enlarged six-pseudostate (E6PS) one [2], still could not account for the loss of dipole polarizability of Ps(1s) that incurred inaccurate results of the cross section for Ps(1s)-p elastic scattering at low energies [3]. In order to get accurate cross sections for both entrance channels, the Ps  $3\overline{p}$  pseudostates should also be included in the coupling scheme to correct the deficiency of its polarization effect more properly. Indeed, the Ps  $3\overline{p}$  pseudostate will, together with the Ps 2p state, also account for 100% of the dipole polarizability of Ps(1s). This further enlarged coupling scheme will, henceforth, be referred to as an enlarged eight state (E8S) [(1s,2s,2p,3p)H-(1s,2s,2p,3p)Ps]+correlationterms] scheme.

The present calculation employs this coupling scheme to reproduce the accurate phase shifts and cross sections that we previously obtained with the E6PS calculation [2] for both  $e^+$ -H and Ps(1s)-p entrance channels. It serves as well to reaffirm that the results of the phase shift and cross section

of our E6PS (and E8PS) calculation have, indeed, approached their "exact" values probably within a few percents. The E8S calculation is also used to supersede the deficient ME6S calculation done previously [3].

#### **RESULTS AND DISCUSSION**

The phase shifts of the E8S calculation for all the partial waves (L=0-6) (see Tables I and II) agree excellently with those of the enlarged six-pseudostate (E6PS) [2] calculation. These results again confirm the predominance of polarization scattering at low energies and higher partial waves  $(L \ge 3)$ . The (numerical) accuracy of the  $L \ge 3$  partial-wave phase shifts at low energies might be further improved somewhat. However, we do not push hard to get this improvement, since these higher-partial-wave cross sections at low energies are very small and their contribution to the total cross sections, as a whole, is, therefore, too insignificant to make this numerical effort worthwhile. The present E8S total cross sections of elastic scattering (Table II), obtained by summing the seven lowest-partial-wave cross sections (L=0-6), agree excellently with those we calculated with the E6PS [2] coupling schemes. The elastic and Ps formation cross sections at energies in the Ore gap calculated with the E8S scheme also agree excellently with those calculated with the E6PS. See Tables III and IV.

For elastic scattering of the Ps(1s)-p entrance channel (Table V), the cross sections calculated with the E8S scheme agree excellently with those we calculated with the E6PS (and E8PS) scheme [2]. Both sets of cross sections at low energies (and especially in higher-partial-wave scattering) deviate considerably from those of the ME6S scheme [3] (that does not include the Ps  $3\overline{p}$  pseudostate). Thus, the inaccuracy of the ME6S Ps(1s)-p results at low energies must obviously originate from the deficiency of the dipole polarizability of Ps(1s).

The total cross sections of H formation calculated with the E8S scheme (Table VI) also agree excellently with those calculated with the E6PS scheme. The scattering lengths of elastic  $e^+$ -H and Ps(1s)-p scattering that we calculate with the E8S and E6PS (Table VII) agree excellently with each other. However, the Ps(1s)-p scattering lengths of both cal-

1332

© 1997 The American Physical Society

TABLE I. *S*, *P*, and *D* wave phase shifts (in units of radians) for positron-hydrogen scattering. Algebraic E6PS [2]: Harris-Nesbet enlarged six-pseudostate  $[(1s,2\overline{s},2\overline{p})H+(1s,2\overline{s},2\overline{p})Ps+correlation terms]$ ; present algebraic E8S: Harris-Nesbet enlarged eight-state  $[(1s,2s,2p,3\overline{p})H+(1s,2s,2p,3\overline{p})Ps+correlation terms]$ . Variational: variational calculation by Bhatia *et al.* [9]. 21 state: 21-state close-coupling approximation by Mitroy and Ratnavelu [11].

$k (a_0^{-1} \text{ units})$	0.1	0.15	0.2	0.3	0.4	0.5	0.6	0.7
			L = 0					
Algebraic E6PS	0.1483	0.1783	0.1876	0.1671	0.1196	0.0621	0.003 29	-0.0520
Present algebraic E8S	0.1482	0.1782	0.1875	0.1671	0.1196	0.0621	0.003 31	-0.0520
21 state	0.1474		0.1868	0.1667	0.1191	0.0621	0.003 1	-0.0518
Variational	0.1483		0.1877	0.1677	0.1201	0.0624	0.003 9	-0.0512
			L = 1					
Algebraic E6PS	0.008 85	0.0192	0.0328	0.0657	0.1003	0.1305	0.1543	0.1785
Present algebraic E8S	0.008 85	0.0192	0.0327	0.0657	0.1002	0.1305	0.1543	0.1784
21 state	0.008 87		0.0327	0.0657	0.1002	0.1306	0.1542	0.1788
Variational			0.0338	0.0665	0.1016	0.1309	0.1547	0.1799
			L=2					
Algebraic E6PS	0.001 33	0.003 04	0.005 49	0.0129	0.0241	0.0396	0.0597	0.0883
Present algebraic E8S	0.001 34	0.003 04	0.005 48	0.0129	0.0241	0.0396	0.0597	0.0884
21 state	0.001 36		0.005 51	0.0129	0.0242	0.0397	0.0598	0.0885

culations deviate considerably from that of the ME6S calculation as expected.

The excellent agreement between the results of our present E8S calculation and those of our previous E6PS calculation [2] is due to the fact that the dipole polarizabilities of both H(1s) and Ps(1s) were taken into account fully in both calculations. We also show for comparison, in the various tables, the *S*- and *P*-wave phase shifts calculated by

Bhatia *et al.* [9], the *S*-, *P*-, and *D*-wave elastic  $e^+$ -H scattering and Ps-formation cross sections by Humberston and co-worker [10], and the phase shifts and cross sections (of both entrance channels) by Mitroy and Ratnavelu [11].

We show the reactance (R) matrix elements of our various calculations for *S*, *P*, and *D* wave scattering in Tables VIII–X. As far as the accuracy of the calculation is concerned, the reactance matrix elements are more informative

TABLE II. L=3, 4, 5, and 6 phase shifts in units of radians and total elastic  $e^+$ -H scattering cross sections in  $\pi a_0^2$  units. Present algebraic 21 state: 21-state coupled-state approximation calculated with the Harris-Nesbet method. Others are the same as in Table I.

$\overline{k \ (a_0^{-1} \text{ units})}$	0.1	0.15	0.2	0.3	0.4	0.5	0.6	0.7
			L=3					
Algebraic E6PS	0.000 435	0.000 990	0.001 77	0.004 06	0.007 50	0.012 5	0.019 7	0.030 5
Present algebraic E8S	0.000 436	0.000 991	0.001 77	0.004 06	0.007 51	0.012 5	0.019 7	0.030 6
21 state	0.000 452		0.001 80	0.004 09	0.007 54	0.012 6	0.019 8	0.030 7
			L = 4					
Algebraic E6PS	0.000 193	0.000 443	0.000 793	0.001 80	0.003 25	0.005 25	0.007 99	0.011 9
Present algebraic E8S	0.000 193	0.000 443	0.000 794	0.001 80	0.003 25	0.005 25	0.008 00	0.012 0
Present algebraic 21 state	0.000 193	0.000 443	0.000 793	0.001 80	0.003 24	0.005 23	0.007 98	0.011 9
21 state	0.000 205		0.000 819	0.001 83	0.003 29	0.005 30	$0.008\ 07$	0.012 1
			L = 5					
Algebraic E6PS	0.000 100	0.000 233	0.000 420	0.000 957	0.001 72	0.002 72	0.004 03	0.005 76
Present algebraic E8S	0.000 100	0.000 234	0.000 421	0.000 959	0.001 72	0.002 72	0.004 03	0.005 77
Present algebraic 21 state	0.000 100	0.000 233	0.000 420	0.000 957	0.001 71	0.002 71	0.004 02	0.005 75
21 state	0.000 109		0.000 443	0.000 986	0.001 75	0.002 77	0.004 10	0.005 87
			L = 6					
Algebraic E6PS	0.000 0570	0.000 136	0.000 247	0.000 566	0.001 01	0.001 60	0.002 34	0.003 26
Present algebraic E8S	0.000 0573	0.000 138	0.000 248	0.000 567	0.001 02	0.001 60	0.002 34	0.003 27
21 state	0.000 0633		0.000 266	0.000 593	0.001 05	0.001 65	0.002 41	0.003 36
		То	tal elastic cros	s sections				
Algebraic E6PS	8.835	5.802	3.818	1.849	1.194	1.023	1.025	1.179
Present algebraic E8S	8.816	5.793	3.814	1.847	1.193	1.023	1.025	1.179
21 state	8.736		3.787	1.844	1.192	1.026	1.026	1.186

TABLE III. Elastic cross sections for positron-hydrogen scattering in  $\pi a_0^2$  units at positron energies in the Ore gap. Variational: variational calculation by Humberston and co-worker [10]. 21 state: 21-state close-coupling approximation by Mitroy and Ratnavelu [11]. Others are the same as in Tables I and II. Numbers in square brackets indicate powers of ten.

$k (a_0^{-1} \text{ units})$	0.71	0.735	0.75	0.80	0.85
		L = 0			
Algebraic E6PS	0.258 [-1]	0.366 [-1]	0.432 [-1]	0.653 [-1]	0.859 [-1]
Present algebraic E8S	0.258 [-1]	0.366 [-1]	0.432 [-1]	0.652 [-1]	0.858 [-1]
21 state	0.258 [-1]		0.430 [-1]	0.657 [-1]	0.849 [-1]
Variational	0.26 [-1]		0.43 [-1]	0.65 [-1]	0.85 [-1]
		L = 1			
Algebraic E6PS	0.802	0.761	0.725	0.625	0.551
Present algebraic E8S	0.802	0.761	0.724	0.625	0.549
21 state	0.802		0.726	0.626	0.551
Variational	0.789		0.724	0.622	0.547
		L=2			
Algebraic E6PS	0.339	0.411	0.444	0.483	0.475
Present algebraic E8S	0.340	0.411	0.444	0.483	0.475
21 state	0.341		0.446	0.484	0.477
Variational	0.323		0.403	0.423	0.413
		L=3			
Algebraic E6PS	0.569 [-1]	0.685 [-1]	0.774 [-1]	0.110	0.134
Present algebraic E8S	0.569 [-1]	0.685 [-1]	0.775 [-1]	0.110	0.134
21 state	0.575 [-1]		0.781 [-1]	0.111	0.135
		L=4			
Algebraic E6PS	0.111 [-1]	0.128 [-1]	0.140 [-1]	0.198 [-1]	0.270 [-1]
Present algebraic E8S	0.111 [-1]	0.128 [-1]	0.141 [-1]	0.198 [-1]	0.271 [-1]
		Total			
Algebraic E6PS	1.239	1.295	1.308	1.311	1.279
Present algebraic E8S	1.239	1.295	1.309	1.311	1.280
21 state	1.242		1.313	1.316	1.285

TABLE IV. Ps(1s)-formation cross sections in  $\pi a_0^2$  units for positron-hydrogen scattering at positron energies in the Ore gap. Same as in Table III.

$\overline{k \ (a_0^{-1} \text{ units})}$	0.71	0.735	0.75	0.80	0.85
		L = 0			
Algebraic E6PS	0.404 [-2]	0.409 [-2]	0.426 [-2]	0.480 [-2]	0.550 [-2]
Present algebraic E8S	0.405 [-2]	0.409 [-2]	0.426 [-2]	0.479 [-2]	0.552 [-2]
21 state	0.405 [-2]		0.427 [-2]	0.472 [-2]	0.560 [-2]
Variational	0.41 [-2]		0.44 [-2]	0.49 [-2]	0.58 [-2]
		L = 1			
Algebraic E6PS	0.267 [-1]	0.297	0.366	0.483	0.563
Present algebraic E8S	0.267 [-1]	0.297	0.366	0.483	0.564
21 state	0.266 [-1]		0.366	0.483	0.563
Variational	0.27 [-1]		0.365	0.482	0.561
		L=2			
Algebraic E6PS	0.682 [-3]	0.145	0.321	0.860	1.158
Present algebraic E8S	0.684 [-3]	0.145	0.321	0.860	1.158
21 state	0.682 [-3]		0.320	0.859	1.158
Variational	0.62 [-3]		0.335	0.812	1.057
		L=3			
Algebraic E6PS	0.445 [-5]	0.948 [-2]	0.357 [-1]	0.271	0.595
Present algebraic E8S	0.446 [-5]	0.949 [-2]	0.357 [-1]	0.271	0.595
21 state	0.44 [-5]		0.356 [-1]	0.270	0.596
		Total			
Algebraic E6PS	0.314 [-1]	0.456	0.730	1.663	2.492
Present algebraic E8S	0.314 [-1]	0.456	0.730	1.662	2.493
21 state	0.313 [-1]		0.728	1.660	2.49

TABLE V. Ps(1s)-p elastic cross sections in  $\pi a_0^2$  units at positron energies in the Ore gap. ME6S [3]: modified enlarged six state [(1s,2s,2p,3p)H-(1s,2s,2p)Ps+correlation terms]. Others are the same as in Tables II and III.

Ps Energy (Ryd)	0.0041	0.040 225	0.0625	0.1400	0.2225
		L = 0			
Algebraic E6PS	59.90	3.285	6.936	9.874	8.335
Algebraic ME6S	58.39	3.394	7.052	9.930	8.366
Present algebraic E8S	60.09	3.278	6.929	9.868	8.331
21 state	59.7		6.92	9.86	8.32
Variational	56.7		7.05	9.93	8.37
		L = 1			
Algebraic E6PS	15.08	10.91	4.103	0.172	1.80
Algebraic ME6S	14.38	10.63	3.928	0.197	1.921
Present algebraic E8S	15.09	10.94	4.114	0.171	1.802
21 state	15.2		4.17	0.160	1.77
Algebraic 21 state	15.03	10.85	4.074	0.173	1.81
		L=2			
Algebraic E6PS	0.7613	6.163	7.014	4.205	1.777
Algebraic ME6S	0.6227	5.94	6.748	4.050	1.646
Present algebraic E8S	0.7616	6.174	7.030	4.214	1.782
21 state	0.792		7.07	4.26	1.82
Algebraic 21 state	0.7603	6.131	6.972	4.183	1.769
		L=3			
Algebraic E6PS	0.112	1.171	1.81	3.27	3.59
Algebraic ME6S	0.750 [-1]	1.080	1.70	3.13	3.39
Present algebraic E8S	0.112	1.172	1.81	3.27	3.60
21 state	0.119		1.85	3.32	3.64
Algebraic 21 state	0.112	1.168	1.80	3.247	3.566
		Total			
Algebraic E6PS	75.89	21.97	20.55	19.14	18.18
Algebraic ME6S	73.49	21.42	20.04	18.79	17.80
Present algebraic E8S	76.10	22.00	20.57	19.16	18.20
21 state	75.9		20.8	19.5	18.6

than the cross sections. Indeed, the deficiency of the scattering effect originating from the closed positronium channels usually can only be recognized in the reactance matrix elements [or in the cross sections of the Ps(1s)-p entrance channel]. As well the deficiency of the polarization effect of a coupling scheme is usually masked in low-partial-wave scattering. Thus, a calculation can be regarded as "accurate in its strict sense" only if it can produce accurate reactance matrix elements, especially for higher-partial-wave scattering and low scattering energies, where the deficiency of the polarization effect of the coupling scheme (or equivalently, trial wave function) is usually not hidden. Through the matrix elements shown, we can, indeed, recognize the deficiency of our ME6S calculation clearly.

TABLE VI. Total H-formation cross sections in units of  $\pi a_0^2$  at positron energies in the Ore gap. Same as in Table III.

Ps Energy (Ryd)	0.0041	0.040 225	0.0625	0.1400	0.2225
		Total			
Algebraic E6PS	1.930	3.060	3.283	3.800	4.047
Present algebraic E8S	1.930	3.060	3.283	3.799	4.048
21 state	1.924		3.28	3.79	4.05

In general, our results of the phase shift and cross section in both  $e^+$ -H and Ps(1s)-p entrance channels agree very well with those calculated by Mitroy and Ratnavelu [11] with the 21-state close-coupling approximation, except for some minor discrepancy found in higher-partial-wave phase shifts and in some cross sections of Ps(1s)-p elastic scattering. It should be noted that, to our knowledge, Mitroy and Ratnavelu [11] are the only research group to have also car-

TABLE VII. Scattering lengths of  $e^+$ -H and Ps(1s)-p scatterings in units of  $a_0$ . Algebraic ECS: enlarged coupled-static [1sH +1sPs+correlation terms] Harris-Nesbet calculation by Gien [2]. Algebraic E6S: enlarged six-state [1s,2s,2p)H+(1s,2s,2p)Ps +correlation terms] Harris-Nesbet calculation by Gien [1,2]. Others are the same as in Table III.

	e <sup>+</sup> -H scattering	Ps(1s)-p scattering
Algebraic ECS	-1.927	-13.69
Algebraic E6S	-2.059	-15.36
Algebraic E6PS	-2.096	-15.86
Algebraic ME6S	-2.101	-14.48
Present algebraic E8S	-2.095	-15.89
21 state	$-2.08 \pm 0.02$	$-15.1\pm0.2$

TABLE VIII. Reactance matrix elements, *S*-wave scattering. 1: H(1*s*) channel, 2: Ps(1*s*) channel. Algebraic E8PS [2]: Harris-Nesbet enlarged eight pseudostate  $[(1s,2\overline{s},2\overline{p},3\overline{d})H + (1s,2\overline{s},2\overline{p},3\overline{d})Ps + correlation terms]$ . Others are the same as in Table V.

withitit	$R_{11}$	$R_{12}$	$R_{22}$
	S wave		
ME6S	-0.05695	$-0.024\ 11$	0.3689
E8S	-0.05696	$-0.024\ 19$	0.3750
E6PS	-0.05699	$-0.024\ 17$	0.3743
E8PS	$-0.056\ 88$	$-0.024\ 16$	0.3748
Variational	-0.057	-0.024	0.363
ME6S	$-0.078\ 50$	$-0.028\ 31$	-0.5321
E8S	$-0.078\ 50$	-0.02774	-0.5262
E6PS	-0.07854	-0.02777	-0.5265
E8PS	-0.07849	$-0.027\ 62$	-0.5265
Variational	-0.078	-0.028	-0.532
ME6S	-0.1040	-0.05125	-1.514
E8S	-0.103 9	$-0.050\ 20$	-1.499
E6PS	-0.1040	$-0.050\ 25$	-1.500
E8PS	-0.103 8	$-0.050\ 27$	-1.499
Variational	-0.104	-0.051	-1.512
ME6S	-0.1294	-0.1224	-3.722
E8S	-0.129 3	-0.1194	-3.611
E6PS	-0.129 3	-0.119 6	-3.624
E8PS	-0.129 1	-0.119 6	-3.614
Variational	-0.130	-0.126	-3.735
	ME6S E8S E6PS E8PS Variational ME6S E8S E6PS E8PS Variational ME6S E8PS Variational ME6S E8PS Variational ME6S E8S E6PS E8PS Variational	$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	$\begin{array}{c c c c c c c c c c c c c c c c c c c $

TABLE IX. Reactance matrix elements, *P*-wave scattering. Same as in Table VIII.

k (a.u.)	Method	$R_{11}$	$R_{12}$	<i>R</i> <sub>22</sub>
		P wave		
0.71	ME6S	0.1868	0.034 29	0.099 95
	E8S	0.1870	0.034 26	0.102 4
	E6PS	0.1870	0.034 26	0.102 4
	E8PS	0.1870	0.034 26	0.102 4
	Variational	0.187	0.034	0.081
0.75	ME6S	0.1938	0.138 9	0.213 1
	E8S	0.1940	0.138 9	0.218 3
	E6PS	0.1941	0.139 0	0.218 0
	E8PS	0.1941	0.138 9	0.218 4
	Variational	0.194	0.139	0.215
0.80	ME6S	0.1870	0.168 2	$-0.059\ 11$
	E8S	0.1873	0.168 0	$-0.053\ 81$
	E6PS	0.1874	0.168 1	$-0.054\ 17$
	E8PS	0.1874	0.168 0	-0.05372
	Variational	0.187	0.168	-0.056
0.85	ME6S	0.1774	0.201 9	-0.2780
	E8S	0.1779	0.201 2	-0.2681
	E6PS	0.1779	0.201 2	-0.2683
	E8PS	0.1781	0.201 1	-0.2678
	Variational	0.177	0.201	-0.273

TABLE X. Reactance matrix elements, *D*-wave scattering. Same as in Table VIII.

k (a.u.)	Method	$R_{11}$	$R_{12}$	<i>R</i> <sub>22</sub>
		D wave		
0.71	ME6S	0.092 79	0.004 167	0.015 98
	E8S	0.092 92	0.004 172	0.017 68
	E6PS	0.092 89	0.004 163	0.017 67
	E8PS	0.092 94	0.004 172	0.017 68
	Variational	0.090 6	0.004 0	0.000 9
0.75	ME6S	0.115 0	0.098 52	0.212 7
	E8S	0.115 2	0.098 76	0.217 3
	E6PS	0.115 2	0.098 74	0.217 1
	E8PS	0.115 2	0.098 76	0.217 4
	Variational	0.109	0.100	0.176
0.80	ME6S	0.133 0	0.177 8	0.254 9
	E8S	0.133 3	0.177 8	0.260 3
	E6PS	0.133 2	0.177 8	0.260 0
	E8PS	0.133 3	0.177 8	0.260 5
	Variational	0.123	0.170	0.210
0.85	ME6S	0.139 5	0.220 6	0.205 1
	E8S	0.140 0	0.220 5	0.213 9
	E6PS	0.140 0	0.220 6	0.213 6
	E8PS	0.140 1	0.220 5	0.214 0
	Variational	0.126	0.207	0.129

ried out the "accurate calculation" for both  $e^+$ -H and PS (1s)-p entrance channels. However, we believe that this discrepancy might just arise from the numerical uncertainty that does seem to exist among the different numerical methods of calculation. To show that such a numerical uncertainty exists, we present in Tables II and V samples of the results of our 21-state coupled-state calculation employing exactly the same coupling scheme as Mitroy and Ratnavelu's but done with the Harris-Nesbet method. Our Harris-Nesbet 21-state (tentative) values are indeed found, in general, to agree better with our E6PS and E8S values than with the 21-state values calculated by Mitroy and Ratnavelu [11] with a different numerical method.

The excellent agreement between the results of our E6PS and E8S calculations, whose enlarged coupling schemes are built on two different basic ones, indicates that the phase shifts and cross sections obtained have approached their "exact" values probably within a few percents. The addition of the H  $3\overline{d}$  and Ps  $3\overline{d}$  pseudostates to our E6PS coupling scheme account for the quadrupole polarization effect more properly in our enlarged eight pseudostate (E8PS)  $[(1s,2\overline{s},2\overline{p},3d)H - (1s,2\overline{s},2\overline{p},3d)Ps + \text{correlation terms}]$  calculation [2] was found to produce virtually unchanged results. This fact indicates that further improvement in accounting for the polarization effect in our calculations is, apparently, not necessary. Finally, it may be worth stressing that our Harris-Nesbet calculations done with enlarged coupling schemes (to get a better accuracy for the cross sections) should (and did) reproduce and enhance the "accuracyindependent" special features [6] of the coupled-state method as expected.

### CONCLUSION

To summarize, Harris-Nesbet calculations with the enlarged E8S scheme also provide accurate results of the phase shift and cross section at low energies for both  $e^+$ -H and Ps(1s)-p entrance channels. The disadvantage of the E8S scheme is that it is more cumbersome than the E6PS one [2]. The E8S calculation, therefore, consumes more computer time. The E8S scheme is, however, useful for studies that require an explicit inclusion of the n=2 H and n=2 Ps states, such as calculations at energies beyond the Ore gap. The present E8S results supersede our ME6S ones obtained previously [3]. The results of our calculations also reaffirm that we have, indeed, attained very accurate values for phase shifts and cross sections in both  $e^+$ -H and Ps(1s)-p entrance channels with our E6PS, E8PS, and E8S Harris-Nesbet variational calculations.

## ACKNOWLEDGMENT

I wish to thank the Natural Science and Engineering Research Council of Canada (NSERCC) for its continual financial support of my research projects, within which this work has been carried out.

- [1] T. T. Gien, J. Phys. B 29, 2127 (1996).
- [2] T. T. Gien, J. Phys. B 30, L23 (1997).
- [3] Y. R. Kuang and T. T. Gien, Phys. Rev. A 55, 256 (1997).
- [4] R. K. Nesbet, Phys. Rev. 175, 134 (1968); 179, 60 (1969); Variational Method in Electron-Atom Scattering Theory (Plenum, New York, 1980).
- [5] K. Higgins and P. G. Burke, J. Phys. B 26, 4269 (1993).
- [6] See, for instance, T. T. Gien, in *The Physics of Electronic and Atomic Collisions*, The Nineteenth International Conference on the Physics of Electronic and Atomic Collisions, Whistler, B.C., Canada, 1995, Abstracts of Contributed Papers, edited by J. B. A. Mitchell *et al.* (ICPEAC, London, Ontario, 1995), Vol. I, p. 360.
- [7] T. T. Gien, in Proceedings of the Positron Workshop 1995, Vancouver, B.C., Canada, 1995 [Can. J. Phys. 74, 343 (1996)].
- [8] P. G. Burke, D. F. Gallaher, and S. Geltman, J. Phys. B 2, 1142 (1969).
- [9] A. K. Bhatia, A. Temkin, R. J. Drachman, and H. Eiserike, Phys. Rev. A 3, 1283 (1971); A. K. Bhatia, A. Temkin, and H. Eiserike, *ibid.* 9, 219 (1974).
- [10] J. W. Humberston, J. Phys. B 17, 2353 (1984); C. J. Brown and J. W. Humberston, *ibid.* 18, L401 (1985).
- [11] J. Mitroy and K. Ratnavelu, J. Phys. B 28, 287 (1995); J. Mitroy, Aust. J. Phys. 48, 645 (1995); 48, 893 (1995).