Coupled-State Calculations of H^+-H Scattering

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A numerical calculation has been performed for proton–hydrogen-atom scattering using $1s$, $2s$, $2p_0$, and $2p_1$ hydrogenic states in a two-center traveling-wave expansion in the impact-parameter method. Discrepancies with past work are pointed out and discussed. Cross sections for direct and exchange scattering into $1s$, $2s$, and $2p$ states, as well as the polarization, are presented for ion energies from 500 eV to 400 keV. Results are compared with other calculations using different expansion functions, both hydrogenic and "pseudostate."

I. INTRODUCTION

Wilets and Gallaher[1,2] (Refs. 1 and 2 are denoted WG and GW, respectively) began a series of papers in which comprehensive studies of the effect of excited states in the two-center traveling-wave expansion were tested in the impact-parameter treatment of proton–hydrogen-atom scattering. In WG, the wave function was expressed as a linear combination of traveling-wave atomic-hydrogen functions, whereas traveling-wave Sturmian functions were used in GW. The contribution of WG lies not only in its completeness and rigor, but in the beautiful use of molecular symmetries, the elucidation of the Coriolis coupling terms for non-s-states, and the exposition of the "invaluable check." The invaluable check is a numerical test of programming accuracy which guarantees conservation of probability if it holds. However, the numerical cross sections and polarizations of WG displayed oscillations at low energies which did not appear reasonable. Since we had already[3] performed the two-state problem (including only $1s$ and $2s$ states on each atom) it was decided to recheck the results of WG. Since that time, a new paper has appeared[4(a)] in which the calculations of WG were repeated, and a new calculation was done including three pseudostates as well as the $1s$, $2s$, $2p_0$, and $2p_1$ hydrogen states in the expansion. It is now clear that the original calculations in WG and GW both contain numerical errors.[4(b)] In the present paper we present new calculations for the $1s/2s/2p_0/2p_1$

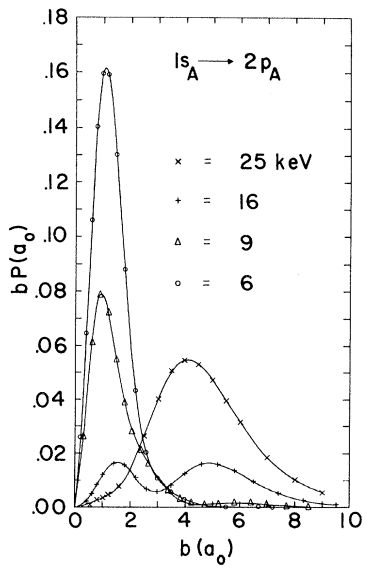

FIG. 1. Plot of (impact parameter) × (probability) vs impact parameter for direct excitation to the $2p$ state at ion energies of 6, 9, 16, and 25 keV.

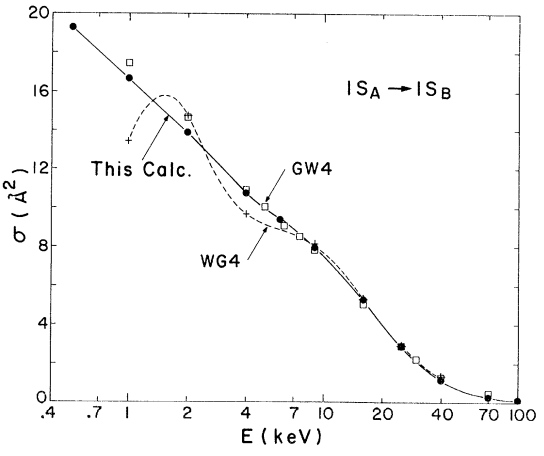

FIG. 2. Cross section vs ion energy for the process $1s_A \rightarrow 1s_B$. The WG4 curve is that calculated in Ref. 1 using a four-state hydrogen expansion. The GW4 points are from the four-state Sturmian calculation of Ref. 2.

TABLE I. Transition probabilities vs impact parameter at 25 keV.

	Direct transitions				Exchange transitions			
$b(a_0)$	$1s$	$2s$	$2p_0$	$2p_1$	$1s$	$2s$	$2p_0$	$2p_1$
0.20	0.225 19	0.014 11	0.002 03	0.000 16	0.733 52	0.023 56	0.001 26	0.000 13
0.30	0.227 93	0.014 81	0.002 12	0.000 28	0.728 37	0.025 14	0.001 07	0.000 24
0.50	0.240 82	0.016 44	0.002 34	0.000 63	0.708 94	0.029 50	0.000 78	0.000 50
0.80	0.285 56	0.017 63	0.002 20	0.001 25	0.656 10	0.036 25	0.000 16	0.000 83
1.00	0.332 80	0.016 90	0.001 94	0.001 71	0.605 95	0.039 71	0.000 00	0.000 96
1.20	0.390 98	0.015 20	0.001 65	0.002 22	0.546 98	0.041 81	0.000 11	0.001 02
1.60	0.524 31	0.010 84	0.001 49	0.003 37	0.416 38	0.041 51	0.000 95	0.001 06
2.00	0.653 85	0.007 24	0.002 36	0.004 62	0.292 29	0.036 25	0.002 08	0.001 17
2.50	0.782 33	0.004 52	0.004 45	0.006 04	0.171 37	0.026 50	0.003 19	0.001 44
3.00	0.868 02	0.003 03	0.006 43	0.006 90	0.092 99	0.017 12	0.003 67	0.001 70
3.50	0.920 43	0.002 13	0.007 43	0.006 98	0.047 52	0.010 07	0.003 54	0.001 75
4.00	0.951 39	0.001 51	0.007 33	0.006 36	0.023 17	0.005 52	0.003 01	0.001 58
4.50	0.969 74	0.001 07	0.006 46	0.005 34	0.010 86	0.002 86	0.002 30	0.001 27
5.00	0.980 82	0.000 75	0.005 26	0.004 20	0.004 92	0.001 42	0.001 61	0.000 93
5.50	0.987 67	0.000 52	0.004 05	0.003 14	0.002 16	0.000 67	0.001 05	0.000 62
6.00	0.992 00	0.000 35	0.003 00	0.002 27	0.000 93	0.000 31	0.000 64	0.000 40
7.00	0.996 53	0.000 15	0.001 54	0.001 10	0.000 16	0.000 06	0.000 21	0.000 14
8.00	0.998 42	0.000 06	0.000 76	0.000 51	0.000 03	0.000 01	0.000 06	0.000 04
9.00	0.999 22	0.000 02	0.000 38	0.000 24	0.000 00	0.000 00	0.000 02	0.000 01
10.20	0.999 64	0.000 01	0.000 14	0.000 11	0.000 00	0.000 00	0.000 00	0.000 00
11.50	0.999 78	0.000 00	0.000 06	0.000 05	0.000 00	0.000 00	0.000 00	0.000 00

hydrogenic expansion. The relationship to previous calculations is discussed at some length.

II. CALCULATION PROCEDURE

The calculation reported in this work is a four-state traveling-wave hydrogenic expansion including $1s$, $2s$, $2p_0$, and $2p_1$ states on each nucleus. The coupled equations for the expansion coefficients are the same as those derived in Eqs. (18)–(20) of WG. Unlike WG, we analytically integrated the matrix elements over another dimension[5] to eliminate numerical evaluation of two-dimensional integrals. Our analysis verified the results of Fennema, [5] and we have subsequently extended his tables to higher states. Gauss-Laguerre quadrature was used to evaluate the one-dimensional integrals. It was found that more points were required at high velocities. A variable number of quadrature points was used ranging from 4 at 1 keV to 14 at 200 keV. For each impact parameter and each velocity, the matrix elements were calculated at a series of points along the trajectory. The starting point was varied from $30a_0$ at low energies to $22a_0$ at high collision energies, where a_0 is the Bohr radius. Two regions were defined, with the spacing between points smaller for the inner part of the collision.

TABLE II. Cross sections for charge transfer (Å^2).

	Direct transitions				Exchange transitions				
E (keV)	$2s$	$2p_0$	$2p_1$	$2p$ TOT	$1s$	$2s$	$2p_0$	$2p_1$	$2p$ TOT
0.50	0.0146	0.0090	0.1556	0.1646	19.303	0.0147	0.0077	0.1558	0.1635
1	0.0125	0.0279	0.2268	0.2547	16.687	0.0136	0.0275	0.2257	0.2533
2	0.0800	0.0115	0.2725	0.2841	13.930	0.0789	0.0117	0.2733	0.2850
4	0.0402	0.1753	0.2705	0.4458	10.795	0.0230	0.1844	0.2486	0.4330
6	0.0265	0.2254	0.2045	0.4299	9.448	0.0637	0.2610	0.1854	0.4464
9	0.0584	0.1377	0.0963	0.2341	7.976	0.1934	0.2223	0.1245	0.3469
16	0.1142	0.0971	0.0519	0.1490	5.310	0.2902	0.1056	0.0722	0.1777
25	0.0967	0.2157	0.1894	0.4051	2.915	0.3457	0.0730	0.0406	0.1136
40	0.1334	0.3163	0.3871	0.7034	1.136	0.2300	0.0527	0.0168	0.0696
70	0.1442	0.4274	0.4797	0.9071	0.264	0.0702	0.0158	0.0030	0.0188
100	0.1165	0.4581	0.4860	0.9441	0.089	0.0240	0.0055	0.0008	0.0062
200	0.0607	0.2951	0.4024	0.6976	0.008	0.0017	0.0003	0.0	0.0003
400	0.0280	0.1195	0.2547	0.3742	0.000	0.0	0.0	0.0	0.0

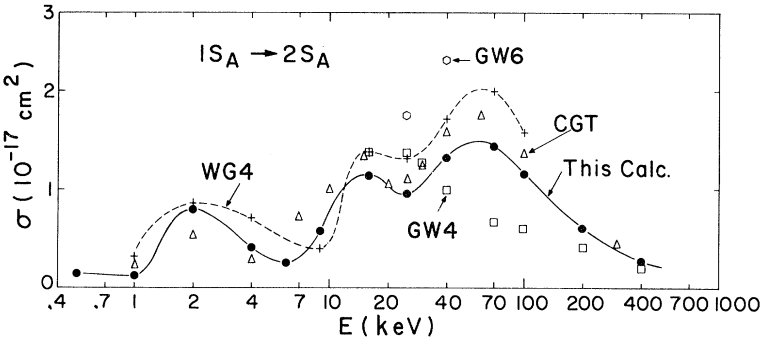

FIG. 3. Cross section vs ion energy for the process $1s_A \rightarrow 2s_A$. Points CGT are from the four-state calculation (CGT4) of Ref. 4. Other notation is same as Fig. 2 and Table III.

Typically the break point between regions was approximately $5a_0$ from the point of closest approach. More points were required at low velocities. A typical calculation utilized 25 points from $-25a_0$ to $-5a_0$, 30 points from $-5a_0$ to $+5a_0$, and 25 points from $5a_0$ to $25a_0$. At each point, the matrix $\hat{G} = \hat{N}^{-1}\hat{H}$ [Eq. (27) of WG] was tabulated. Time-reversal properties of the integrals were used to reduce the amount of calculation by a factor of 2 using symmetry about $t = 0$. The coupled equations were integrated by means of a modified predictor-corrector procedure, the coefficients at any time being determined by interpolation between the points of the $\hat{G}$ matrix, and using Eq. (29) of WG,

$$G_{kk'} = \hat{G}_{kk'} e^{i(\epsilon_k - \epsilon_{k'})t},$$

to obtain the G matrix. In the predictor-corrector integration procedure, the time interval was halved several times on the approach part of the collision, and was doubled several times as the protons separated. The norm of pse was calculated at each time step and was held to 1.0000 ± 0.0001 or better at each step, except for small impact parameters at low velocities. The invaluable check was thoroughly tested. Other possible sources of error are the Coulomb integrals and the normalization constants of the wave functions. (The invaluable check is independent of these quantities.) Tests were made in which the integration parameters were varied over reasonable ranges. The number of storage points for the G matrix was varied from 60 to 100, the number of Gauss-Laguerre integration points was increased by several points, and the starting point was varied by increasing it up to $40a_0$. Small variations in the calculated probabilities occurred which were generally less than ± 0.0003. The probabilities reported in this paper are probably accurate to ± 0.0005, and the cross sections are probably accurate to ± 0.001 Å^2.

III. RESULTS

The probabilities were calculated at approximately 20 impact parameters for each collision velocity. A set of values of probability vs impact parameter for one energy (25 keV) is given in Table I. Similar tables for other energies are available from the authors. Plots of bP vs b were generated by computer on a Calcomp plotter. It was found that several processes could be distinguished. For p states, excitation apparently takes place by one process (probably rotational coupling) at small impact parameters and by another process (probably direct coupling) at large impact parameters. The inner process is favored at low

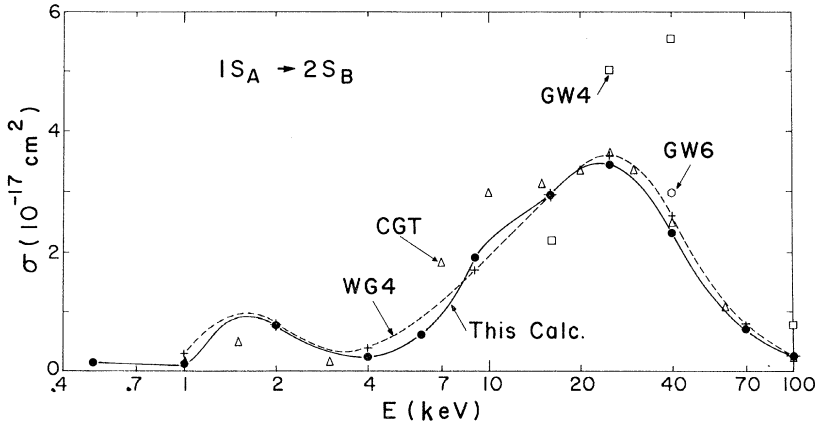

FIG. 4. Cross section vs ion energy for $1s_A \rightarrow 2s_B$. Notation as in Figs. 2 and 3.

TABLE III. List of proton-hydrogen scattering calculations.

states nucleus	Expansion functions	Ref. No.	Ref. Code
1	$1s$ (hydrogenic)	6	M
		3	S1
2	$1s/2s$ (hydrogenic)	3	S2
4	$1s/2s/2p_0/2p_1$	1	WG4
	(hydrogenic)	4	CGT4
		This work	TW
7	$1s/2s/2p_0/2p_1/3s/3p_0/3p_1$ (hydrogenic)	1	WG7
7	$1s/2s/2p_0/2p_1/3\bar{s}/3\bar{p}_0/3\bar{p}_1$ (hydrogenic plus pseudo)	4	CGT7
Various	$1s/2\bar{s}/2p_0/2p_1/3\bar{s}/\ldots$ (Sturmian)	2	GW

velocities and the outer process is favored at high velocities. This is clearly illustrated in Fig. 1 where bP is plotted vs b for collision energies of 6, 9, 16, and 25 keV, and P corresponds to direct excitation to the $2p$ state (sum of $2p_0 + 2p_1$). At 6 keV, the outer process is completely negligible, and at 25 keV, the inner process is very unimportant. Both peaks are clearly in evidence at 16 keV. Similar results are found for exchange transitions. There is also some evidence for two peaks with different energy dependence in the bP vs b curves

TABLE IV. Comparison of cross sections of this work with the $1s/2s/2p_0/2p_1$ results of Ref. 4.

$1s$ exchange cross sections (Å^2)		
E (keV)	This work	$C, G,$ and T
0.5	19.30	
1.0	16.69	16.60
2.0	13.93	14.12
4.0	10.80	10.81
6.0	9.45	
7.0		8.964
9.0	7.98	
10.0		7.591
15.0		5.719
16.0	5.31	
20.0		3.873
25.0	2.92	2.984
30.0		2.145
40.0	1.14	1.169
60.0		0.421
70.0	0.26	
100.0	0.089	0.092
200.0	0.008	
300.0		0.0015
400.0	0.000	

TABLE IV. (*Continued*)

$2s$ hydrogen cross sections (10^{-17} cm^2)				
	Exchange		Excitation	
E (keV)	This work	$C, G+T$	This work	$C, G+T$
0.5	0.147		0.146	
1.0	0.136	0.2259	0.125	0.2221
2.0	0.789	0.5284	0.800	0.5540
4.0	0.230	0.2025	0.402	0.2465
6.0	0.637		0.265	
7.0		1.840		0.7475
9.0	1.93		0.584	
10.0		2.985		1.025
15.0		3.123		1.343
16.0	2.90		1.142	
20.0		3.327		1.076
25.0	3.46	3.655	0.967	1.130
30.0		3.378		1.254
40.0	2.30	2.480	1.334	1.591
60.0		1.125		1.763
70.0	0.702		1.442	
100.0	0.240	0.2633	1.165	1.371
200.0	0.017		0.607	
300.0		0.0033		0.4302
400.0	0.000		0.280	

$2p$ hydrogen cross sections (10^{-17} cm^2)				
	Exchange		Excitation	
E (keV)	This work	$C, G+T$	This work	$C, G+T$
0.5	1.635		1.646	
1.0	2.533	2.436	2.547	2.439
2.0	2.850	3.128	2.841	3.105
4.0	4.330	4.228	4.458	4.543
6.0	4.464		4.299	
7.0		3.320		3.370
9.0	3.469		2.341	
10.0		2.610		1.584
15.0		1.522		1.141
16.0	1.777		1.490	
20.0		1.085		1.816
25.0	1.136	0.924	4.051	3.440
30.0		0.812		4.734
40.0	0.696	0.572	7.034	6.905
60.0		0.242		8.296
70.0	0.188		9.071	
100.0	0.062	0.053	9.441	8.618
200.0	0.003		6.976	
300.0		0.001		4.989
400.0	0.000		3.742	

for the $2s$ state. However, the peaks are closer together and less obviously separate.

It is difficult to elucidate the reaction path (flow of probability) during a collision because of coupling of the $2s$ state with the $2p$ states. One comparison that is interesting is the relation between results of a $[1s_A/1s_B/2s_A/2s_B]$ calculation[3] with $[1s_A/2s_A \text{ or } 2s_B]$ $[1s_A/2s_A/2s_B]$, and $[1s_A/1s_B/2s_A]$

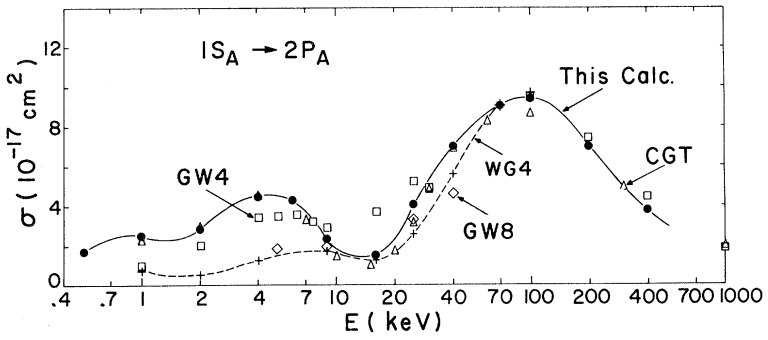

FIG. 5. Cross section vs ion energy for $1s_A \rightarrow 2p_A$. Notation as in Figs. 2 and 3.

calculations,[6] where the $2p$ states are omitted. If these expansions are denoted as 1122, 12, 122, and 112, respectively, the following is found[3] at 5 keV:

For exchange, 112 agrees well with 1122 at all b, whereas 12 and 122 agree with each other but are substantially different from 1122.

For direct excitation, 12 and 122 agree well with 1122 at large b, but fail badly at small b. However, at small b, 112 approaches 1122 but fails at large b.

From these results, it may be concluded that $1s_A \rightarrow 1s_B \rightarrow 2s_B$ is very important, whereas $1s_A \rightarrow 2s_B$ and $1s_A \rightarrow 2s_A \rightarrow 2s_B$ are unimportant, at least at 5 keV. Production of $2s_A$ occurs primarily by $1s_A \rightarrow 2s_A$. The only role that $1s_B$ plays in formation of $2s_A$ is to remove probability from $1s_A$ at times during the collision.

A comparison of two-state ($1s/2s$) results[3] and the present four-state ($1s/2s/2p_0/2p_1$) results indicates that $1s_A \rightarrow 2s_A$ and $1s_A \rightarrow 1s_B \rightarrow 2s_B$ are the dominant processes for formation of the $2s$ states. However, there are enough differences in the $2s$ cross sections calculated by these methods to indicate that processes such as $1s \rightarrow 2p \rightarrow 2s$ and $1s \rightarrow 2s \rightarrow 2p$ are roughly $\frac{1}{3}$ as important as $1s \rightarrow 2s$ and $2s \rightarrow 1s$.

The cross sections were obtained by integrating the bP-vs-b curves and are given in Table II. They are plotted in Figs. 2–6. It can be seen that the exchange cross sections fall off more rapidly than the excitation cross sections at high energies. The calculated values of the polarization, given by $(\sigma_{2p_0} - \sigma_{2p_1})/(\sigma_{2p_0} + \sigma_{2p_1})$, are given in Fig. 7.

IV. DISCUSSION

The various calculations of proton-hydrogen scattering are summarized in Table III. Let us consider the results of these calculations for the process $1s_A \rightarrow 1s_B$. The results of calculations S1 and S2 show that the calculated cross sections for $1s_A \rightarrow 1s_B$ are roughly independent of whether the $2s$ states are included. It appears that all the calculations should give approximately the same results for the $1s_A \rightarrow 1s_B$ process.

The results of TW and Cheshire, Gallaher, and Taylor (CGT4) are compared in Table IV. For the $1s_A \rightarrow 1s_B$ transition, the agreement is very good. On the other hand, the results of WG4 appear to be seriously in error as shown in Fig. 2. The $1s_A \rightarrow 1s_B$ results of GW4 are also consistent with TW. It is difficult to understand why the cross section for $1s_A \rightarrow 1s_B$ are changed by as much as 10% in going from CGT4 to CGT7. For example, at 1 keV, CGT find cross sections for $1s_A \rightarrow 1s_B$ of 19.12 and 16.60 Å^2 from CGT7 and CGT4 calculations, respectively.

The calculated cross sections for production of $2s$ and $2p$ states are compared in Figs. 3–6 and Table III. It can be seen that there is only crude agreement between calculations TW and CGT4. The results of WG4 are known to contain numerical errors at low energies.[4(a)] The GW results using Sturmian functions have poor convergence characteristics. It is not clear why there is a remaining discrepancy between the results of TW and CGT4 for the $n=2$ states. One of the calculations (or both) must contain numerical errors.

The only sources of error we can think of are (a) possibly in the Coulomb integrals, and (b) errors due to the choice of starting point for time

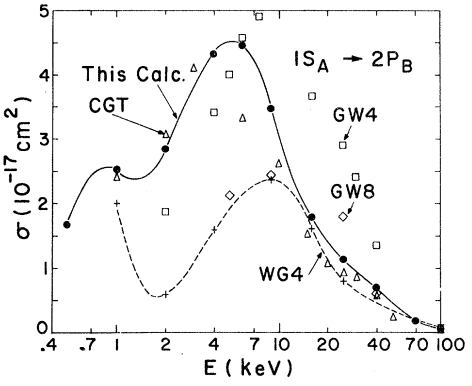

FIG. 6. Cross section vs ion energy for $1s_A \rightarrow 2p_B$. Notation as in Figs. 2 and 3.

TABLE V. Variation of probabilities with starting point at 25 keV and $1a_0$.

Start point (a_0)	$1s(A)$	$2s(A)$	$2p_0(A)$	$2p_1(A)$	$1s(B)$	$2s(B)$	$2p_0(B)$	$2p_1(B)$
20.8	0.3333	0.0167	0.0022	0.0018	0.6057	0.0392	0.0000	0.000 96
22.9	0.3331	0.0168	0.0020	0.0017	0.6059	0.0395	0.0000	0.000 95
25.0	0.3328	0.0169	0.0020	0.0017	0.6059	0.0397	0.0000	0.000 96
27.0	0.3326	0.0169	0.0021	0.0017	0.6060	0.0398	0.0000	0.000 97
29.1	0.3325	0.0169	0.0023	0.0017	0.6060	0.0398	0.0000	0.000 97

integration. The variation of our results with starting point is illustrated in Table V for 25 keV and $1a_0$.

The changes observed upon increasing the starting point beyond $25a_0$ are within the estimated error given at the end of Sec. II. Small changes in $1s(A)$ and $2p_0(A)$ do not affect the cross sections appreciably. Our Coulomb integrals are the same as those given by Fennema, [5] but we cannot compare with CGT because they do not specify their Coulomb integrals.

It is unfortunate that the polarizations resulting from CGT4 were not published. Since papers WG and GW contain numerical errors, it is difficult to evaluate the polarizations reported therein. Fite and co-workers[7] compared their experimental results for polarization in direct excitation of the $2p$ state with the four-state Sturmian results of GW4. Since these calculations are dubious, we have represented the experimental results in Fig. 8 together with our prediction from Fig. 7. Our calculations do not fit Fite's data much better than GW4. This might be due to an inadequacy in the $1s/2s/2p_0/2p_1$ calculation or to errors in the data.

Another interesting comparison is with the calculation of Gaussorgues and Salin[8] who used the low-velocity approximation[3] of neglecting the traveling-wave terms in the expansion functions. They used a $1s/2s/2p_0/2p_1$ procedure similar to the present work, except for omission of the traveling-wave terms. A comparison of the low-velocity calculation including only $1s$ states with the $1s$ calculation including traveling-wave terms was given by Storm[3] and by McCarrol. [9] At ion energies below about 2 keV, there is substantial agreement between the probabilities except at small impact parameters. The cross sections agree at low ion energies, and begin to diverge significantly above 2 keV. The comparison of cross sections for the $2s$ and $2p$ states states in the $1s/2s/2p_0/2p_1$ calculations, with and without the traveling-wave terms in the expansion functions, is given in Figs. 9 and 10. It appears that the low-velocity approximation gives high results for cross sections for $n=2$ states at energies in excess of about 700 eV.

Finally, we wish to discuss the question of convergence of the expansion in hydrogenic orbitals. It is clear from comparison of papers S1, S2, and TW that the cross section for $1s_A \rightarrow 1s_B$ is approximately converged at moderately low energies simply by including only the $1s$ states in the expansion. This can be understood by noting that at low energies, the region of b which determines the magnitude of σ for $1s_A \rightarrow 1s_B$ corresponds to large impact parameters where the probabilities for excitation to $n=2$ states are small. At high energies (>25 keV), however, the probabilities for excitation of the $n=2$ states became more comparable to that for the $1s_B$ state, and there are small differences between the results of S1, S2, and TW. For energies below about 25 keV, the $1s_A \rightarrow 1s_B$ transition appears to be fully converged. The use of three pseudostates in CGT7 changes the calculated cross section markedly from CGT4 at 1 keV. They report for the $1s_A \rightarrow 1s_B$ transition at 1 keV, $\sigma = 19.12$ Å^2 in CGT7 and $\sigma = 16.60$ Å^2 in CGT4, a difference of about 10%. Since the important range of impact parameters for the $1s_A \rightarrow 1s_B$ transition at 1 keV is

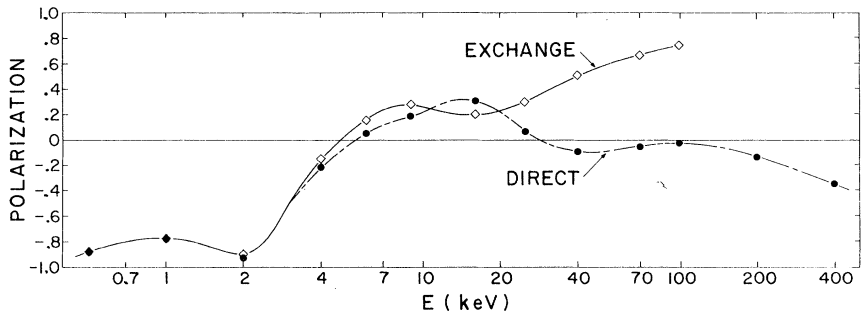

FIG. 7. Polarization $[(\sigma_{2p_0} - \sigma_{2p_1})/(\sigma_{2p_0} + \sigma_{2p_1})]$ vs ion energy for direct excitation and exchange transitions to the $2p$ state.

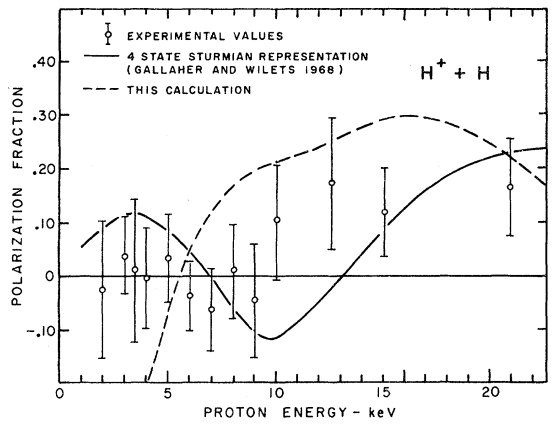

FIG. 8. Comparison of polarizations calculated in this work and in the four-state Sturmian (Ref. 2) with the data of Ref. 8.

$3-7a_0$, it is hard to see why the pseudostates affect this transition so drastically.

The convergence of the hydrogenic expansion for transitions to the $n=2$ states is not nearly so clear as for the $1s_A \rightarrow 1s_B$ transition. In order to test the convergence of the calculation with respect to the $n=2$ states, one would have to perform a calculation including the $n=3$ states. Wilets and Gallaher[1] performed a limited number of such calculations at a few energies. However, their results, as pointed out earlier, contain numerical inaccuracies. If it can be assumed that the nature of these errors is such that the relation between the WG7 and WG4 calculations is correctly represented (i.e., they are both in error by the same amount) then a limited test of the convergence of the hydrogenic expansion can be made. The WG4 and WG7 results are in nearly perfect agreement at 9 and 25 keV for the $2p$ states (both direct and exchange). For the $2s$ states, there is again very good agreement at 25 keV, but the agreement is poor at 9 keV. However, 9 keV is an energy for which the errors in the WG work are expected to be important, whereas at 25 keV the errors appear to be less severe. Therefore, as far as can be discerned from the limited data available, the convergence of the cross sections appears to be quite good for the $n=2$ states in the $1s/2s/2p_0/2p_1$ calculation. It is therefore somewhat surprising to us that CGT[4] in the second sentence of their paper claim that "Wilets and Gallaher[1] ... demonstrated that this expansion is slowly convergent." At 25 keV, the convergence appears very rapid to us. In order to further test this point, we have begun a program to repeat the WG7 calculations using the same method as in TW. However, even though the cross sections might converge, the probabilities at small impact parameter probably do not converge very well. The convergence of the calculations involving Sturmian wave functions is rather slow, as can be seen in Figs. 2–6 of this paper. CGT[4] claim that CGT7 fits the total-charge-exchange-cross-section data better than CGT4.[10] Since the total charge exchange was only measured in the range above 5 keV, and CGT4 and CGT7 agree within a few percent for the total exchange in this energy range, it

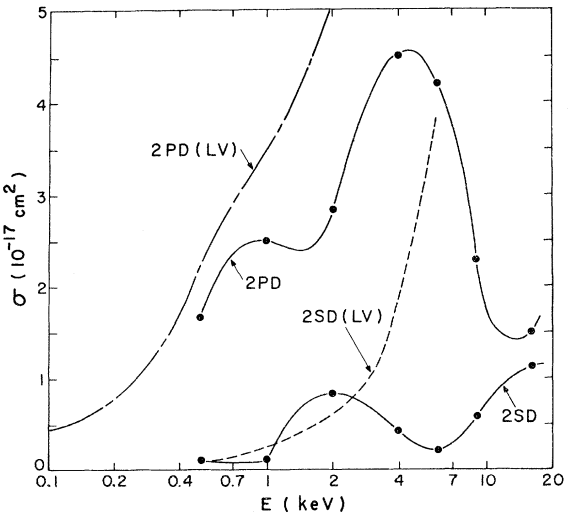

FIG. 9. Comparison of cross sections in the present work with those of Ref. 9 for direct transitions to $n=2$ states.

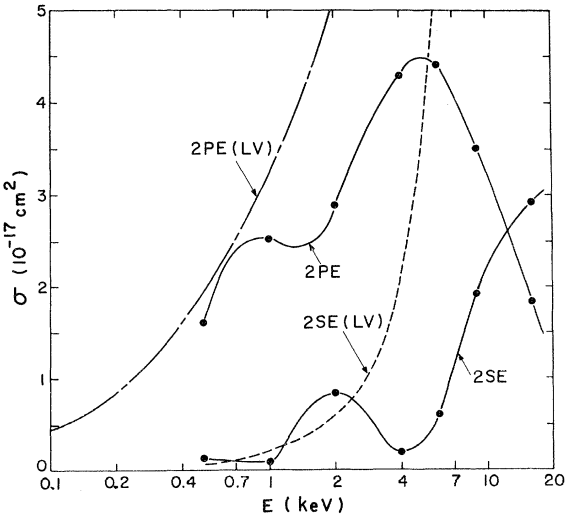

FIG. 10. Comparison of cross sections in the present work with those of Ref. 9 for exchange transitions to $n=2$ states.

is difficult to understand this claim. The convergence of CGT7 could only be tested by adding more states and comparing with CGT7. However, this might involve severe difficulties in projection onto the hydrogen states at infinite separation, including the neglect of "oscillating terms" as is done in the Sturmian calculation.

V. CONCLUSIONS

The following conclusions summarize the findings of this paper:

(i) A numerical calculation of proton-hydrogen scattering has been performed with $1s$, $2s$, $2p_0$, and $2p_1$ hydrogenic states included in the expansion. Numerical errors are definitely present in Refs. 1 and 2. A discrepancy still remains between the present work and that of Ref. 4, which is not yet resolved.

(ii) It appears that the present calculation might be fully converged for purposes of calculating cross sections, at least at moderately high energies. We are presently carrying out similar calculations including $n = 3$ states to test this hypothesis.

(iii) For very small impact parameters, the present calculation is probably far from converged. Attempts by others to use pseudostates to correct for this nonconvergence introduce other difficulties. It is not clear how a good calculation can be accomplished for $b = 0$, with the usual two-centered expansion.

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[4](a) I. M. Cheshire, D. F. Gallaher, and A. J. Taylor, J. Phys. B 3, 813 (1970); (b) L. Wilets (private communication).

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[10]Below Table IV of Ref. 4 appears the passage, "In general we can conclude ... that the inclusion of the pseudostates considerably improves the wave function as the quantities derived from them are closer to the experimental results where these are available. In particular the total charge exchange seems to have converged to the experiments."