Electron transfer, excitation, and ionization in p-H(1s) collisions studied with Sturmian bases

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(Received 13 July 2009; published 2 September 2009)

Cross sections have been determined for electron transfer, direct excitation, and ionization in collisions between protons and H(1s) atoms at proton energies from 1 keV to 16 MeV, extending the pioneering work by Shakeshaft [R. Shakeshaft, Phys. Rev. A **14**, 1626 (1976); Phys. Rev. A **18**, 1930 (1978)] with a much smaller basis and energy range, and following the author's work for other collisional systems [T. G. Winter, Phys. Rev. A **76**, 062702 (2007)]. Transfer as well as excitation cross sections into individual states up to 3d (excitation up to 4f at the higher energies) have been determined with several coupled-Sturmian-pseudostate bases, and tests of basis sensitivity have been carried out. These and ionization cross sections have been compared with experimental, other coupled-state, and numerical results. Ionization and excitation cross sections have also been compared with corresponding Born results at higher energies.

DOI: 10.1103/PhysRevA.80.032701 PACS number(s): 34.70.+e, 34.50.Fa

I. INTRODUCTION

Electron transfer, excitation, and ionization in collisions between protons and hydrogen atoms are fundamental atomic collision processes. At intermediate collision velocities on the order of the Bohr velocity $v_o=c/137$, all three processes can have large cross sections, at least comparable to the Bohr area $\pi a_o^2=8.8\times10^{-17}$ cm^2 and therefore compete. (A proton moving at v_o has a kinetic energy of 25 keV.) See Fig. 1. Accordingly, coupled-state approaches, such as the coupled-atomic-state approach for electron transfer introduced by Bates [1] in 1958, are appropriate. This approach was first carried out by McCarroll [2] in 1961 in a two-atomic-state approximation and yielded good results for capture to the ground state. By the early 1970s, several researchers, including Cheshire *et al.* [3], as well as Winter and Lin [4], extended these calculations to include a limited number of excited *bound* atomic states centered on the projectile and/or target nucleus, providing also cross sections for capture and excitation to lower excited states, but of questionable convergence.

At about the same time and into the late 1970s, ionization began to be included by means of pseudostates, notably by Cheshire *et al.*, Gallaher and Wilets [5], and Shakeshaft [6–8]. The present work closely follows the basic method (but not numerical approach) of Shakeshaft [7] with a Sturmian-pseudostate basis and, indeed, has been extended by the author over 30 years to treat other collisions [9,10]. Although still widely cited as *the* Sturmian calculations for p-H collisions, Shakeshaft's work was necessarily limited in scope by then-available computers, preventing an approach to completeness (as is otherwise in principle possible with a systematic basis such as a Sturmian basis) and preventing an extension to high and, particularly, low collision energies (where comparison with then-existing molecular-state results could have been made [11–14]).

In the 1980s and 1990s, larger coupled-molecular-, as well as coupled-atomic-state, calculations were reported: notably, a 94-atomic-plus-pseudostate calculation with an even-tempered basis by Kuang and Lin [15], a 394-Gaussian-pseudostate calculation by Toshima [16], and a large one-center-pseudostate calculation with a basis of complex Slater orbitals by Ford *et al.* [17]. Kimura and Thorson [18] carried out a ten-molecular-state calculation with optimized translation factors, a calculation greatly expanded to 362 states in 2002 by Zou *et al.* [19]. Following Anderson *et al.* [20], Winter and Lin [21,22] combined the atomic and the molecular approaches by means of a triple-center 36-atomic-state basis, slightly expanded by McLaughlin *et al.* [23] with four additional states on the third center.

It is now possible to carry out a fairly definitive Sturmian calculation for p-H collisions. In addition to establishing much more converged cross sections for capture and excitation to lower excited states at least up to 3d, and over a much wider energy range, one can now address several specific problems. First, an existing coupled-state calculation has predicted that, at low energies, the 2p capture and excitation

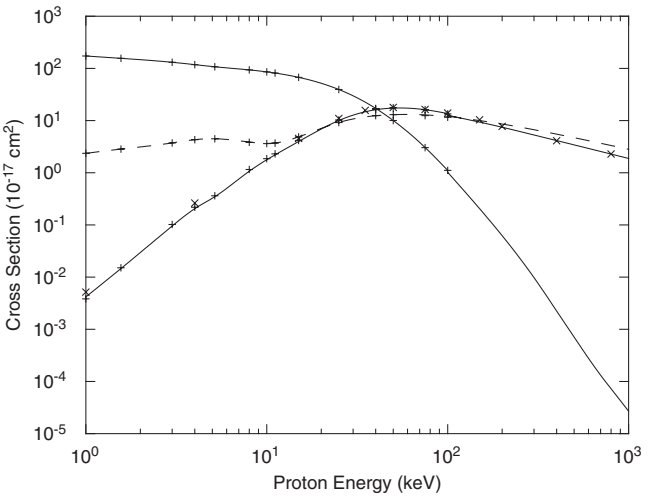

FIG. 1. Coupled-state cross sections for total electron transfer, total direct excitation, and ionization in p-H collisions. The curves from top to bottom on the left are for capture, excitation, and ionization. Curves: 176 Sturmians up to 100 keV, 281 Sturmians at higher energies. Plus signs, 220 Sturmians; crosses, 394 Gaussians [16]. The capture curve at energies of at least 100 keV is for 1s capture, multiplied by 1.202. The Sturmian results are present results with the bases to be described.

cross sections are different [23]; it has been pointed out by Lin [24] and by the author in a recent review paper [25] that this is unphysical. Second, at intermediate energies, the $n=3$ (Balmer-alpha) experimental excitation cross section [26] differs widely from most existing theoretical results [17,27]. Third, at intermediate energies near the peak in the ionization cross section at about 50 keV, it has been noted to be difficult [28] to obtain very accurate theoretical ionization cross sections to compare with the experimental results [29].

The present results are also applicable to other symmetric one-electron heavy-particle collisions with common nuclear charge Ze, such as He^{2+}-He^{+} [30,31], since, within the straight-line impact-parameter approach, cross sections scale exactly as $Q(v,Z)=Q(v/Z,1)/Z^2$, where v is the projectile velocity [32].

The outline of the paper is as follows. In Sec. II, the Sturmian method will be summarized, the results will be presented and compared with the Sturmian results of Shakeshaft, and their accuracy will be assessed. In Sec. III the largest-basis Sturmian results will be compared with other coupled-state results, numerical results [33], first Born results for excitation and ionization [34], and numerous experimental results. Conclusions will be drawn in Sec. IV.

II. METHOD

In essence, in both the present work and that of Shakeshaft [7,8] on which it rests, the Sturmian basis functions on each nucleus are simply polynomials in the radial electronic variable r multiplied by a *fixed* exponential e^{-cr} (as well as a spherical harmonic). The polynomials and hence the Sturmians form a complete set. In the first of the just-cited papers by Shakeshaft and in the author's work, the choice $c=Z/[(\ell+1)a_o]$ is made, so that each of the lowest states $1s,2p,3d,\ldots$ of different angular momenta ℓ can be represented by a single Sturmian (Laguerre function with exponential independent of n); for p-H collisions, we have $Z=1$. In the second just-cited paper, Shakeshaft chose ℓ-dependent smaller values of c to improve the convergence of the basis; the resulting functions, which he called scaled-hydrogenic functions, could also be called scaled-Sturmian functions. The numerical details in Shakeshaft's and the author's work are quite different. Notably, Shakeshaft took full account of the nuclear symmetry to halve the number of states simultaneously coupled and time reversal to halve the number of matrix elements calculated. These improvements in efficiency were not made in the author's computer code, which had been written for the more general heteronuclear case. However, the author did modify the code to cut the number of distinct matrix elements required at each time step. These and other changes at least halve the computing time from that with the heteronuclear code.

A. Numerical tests

1. Integration parameters

As noted in the author's previous work [9,10], several parameters affect the accuracy of the cross sections: (1) the truncation-error limits e_1,e_2 and (2) the limits $z_{\min},z_{\max}$ in integrating the coupled equations over $z=vt$, (3) the limiting internuclear distance $R_{\max}$ and (4) the number of integration points N_λ,N_μ in evaluating the charge-exchange matrix elements in spheroidal coordinates, and (5) the impact parameters ρ in integrating probability times ρ to obtain the cross section. For proton energies of 3, 15, 50, and 100 keV, tests have been made of the sensitivity of cross sections to a choice of these parameters. Coupled-Sturmian cross sections have been determined using the limited basis $\leq 7(s,p,d)$ on each center (68 states in all, with the highest s state on each center neglected after diagonalizing the atomic Hamiltonians) with the reference parameters $e_1,e_2=10^{-7,-5}$, $z_{\min}=-100a_o$, $z_{\max}=1000a_o$, $R_{\max}=70a_o$, $N_\lambda=32$, $N_\mu=40$, and $\rho=0(0.3)3.6(0.6)\rho_{\max}$ (in units of a_o), where $\rho_{\max}=10.8a_o$ at the lower energies, increasing to $20.4a_o$ at 100 keV. The parameters have then been varied to the more stringent values $e_1,e_2=10^{-8,-6}$, $z_{\min}=-200a_o$, $z_{\max}=2000a_o$, $R_{\max}=100a_o$, $N_\lambda=36$, $N_\mu=80$, and $\rho=0(0.15)3.6(0.3)\rho_{\max}+4.8a_o$. The individual cross sections for excitation and transfer to the $2s,2p,3s,3p,3d$ states, as well as for $1s$ and total capture, total excitation, and ionization, have been monitored and no sensitivity exceeds 0.6%, except for greater sensitivity primarily to N_λ,N_μ (up to 6% in one case) for some small $n=3$ cross sections at 3 and 100 keV. These parameters are similar to, or more stringent than, those used in previous work [10]. When a more exacting test is made or when a larger (production) basis is used, then more stringent parameters, notably larger $R_{\max},N_\lambda,N_\mu$, are sometimes chosen. The choice $e_1,e_2=10^{-7,-5}$ is made throughout unless otherwise noted.

2. Summed cross section

An independent test of sensitivity to the parameters has also been monitored. Since the probability should be conserved (unitarity) in integrating the coupled equations, the summed cross section ΣQ (including the elastic channel) should be identical to $\pi\rho_{\max}^2$, but it is not, due to small numerical errors. In the tests carried out above, the *relative* error in ΣQ does not exceed 4×10^{-6}. The *absolute* error in ΣQ is consistent with the absolute sensitivity in the individual cross sections, although in some cases—notably at large impact parameters—the absolute sensitivity is mainly confined to the (large) elastic cross section. The error in ΣQ, monitored in this way, reflects the choice of $e_1,e_2,R_{\max},N_\lambda,N_\mu$, but only indirectly the choice of ρ or the range of z.

3. Highest s state

Following Shakeshaft's 70-scaled-Sturmian calculation [8], the present calculations neglect the highest s state on each center after diagonalizing the atomic Hamiltonian, at least for the larger production bases. This approximation has been tested at 15 keV for the basis $\leq 15(s,p,d)$ on each center. Cross sections are affected by $\leq 0.5\%$ for each state through $n=3$, except 1% for $3p,3d$ capture. The CPU savings is a factor of 2. Other tests have also been performed.

B. Comparison with Shakeshaft's Sturmian results

1. Symmetric s,p basis

Coupled-Sturmian cross sections for excitation and electron transfer in 15–200 keV p-H collisions are given in Table

TABLE I. Coupled-Sturmian cross sections (in units of 10^{-17} cm^2) for excitation and electron transfer in p-H collisions using the basis $\leq(6s,4p)$ on each proton, following Shakeshaft [7]. Numbers in parentheses are differences in the last digit from Shakeshaft's results with the same basis. The asterisks indicate cross sections differing slightly with different parameters.

E	Excitation			Transfer			
(keV)	$2s$	$2p_o$	$2p_1$	$1s$	$2s$	$2p_o$	$2p_1$
15	0.968*(−2)	1.31(−1)	1.59(0)	57.5(0)	3.40(−1)	1.26(1)	1.93(1)
20	1.89(0)	1.84(0)	1.64(0)	41.7(0)	4.21(0)	0.959(3)	1.26(1)
25	2.22(0)	1.99*(1)	2.05(1)	30.1(−1)	4.22(0)	0.709(0)	0.841(5)
35	1.75(1)	2.02(1)	3.50(1)	16.0(0)	3.08*(0)	0.452*(0)	0.424(2)
40	1.43(0)	2.30(−1)	4.16(0)	11.8(0)	2.47(0)	0.364*(0)	0.313(2)
45	1.28(0)	2.76(−1)	4.62(0)	8.85(0)	1.94(0)	0.288(0)	0.234(1)
55	1.49(0)	3.70(0)	4.95(0)	5.18(0)	1.18(0)	0.175(0)	0.132(0)
60	1.67(0)	3.92(1)	4.93(0)	4.04(0)	0.921(1)	0.137(0)	0.0998(4)
70	1.77(0)	3.76*(1)	4.84(0)	2.53(0)	0.573(1)	0.0831(0)	0.0577(2)
125	0.811(−2)	2.60*(1)	4.89*(1)	0.331(0)	0.0675(0)	0.00936(0)	0.00555(0)
200	0.551(−2)	1.97*(2)	4.26*(0)	0.0493(1)	0.00921*(5)	0.00113*(3)	0.00054(1)

I using the basis $\leq(6s,4p)$ on each proton (24 states in all), following Shakeshaft [7] with the same basis (here, with the highest s state fully retained). As a check on their numerical accuracy, the present cross sections have been calculated using two stringent sets of parameters [35]; only those marked with an asterisk differ (the more accurate results being listed), and these by only 1 unit in the last digit, except for a 2 unit difference for $2s$ transfer at the highest energy. The absolute error in the summed cross section is small: $|\Sigma Q-\pi\rho_{\max}^2|\leq 0.000\,01\times10^{-17}$ cm^2 for $E\geq 35$ keV and $\leq 0.0001\times10^{-17}$ cm^2 at lower energies and may independently confirm the sufficiency of the chosen parameters $e_1,e_2,R_{\max},N_\lambda,N_\mu$. The noted differences from Shakeshaft's results are zero or small: rarely do they exceed 1 unit in the last digit, and when they do, they are $\leq 1\%$, except 3% for $2p_0$ at 200 keV. Thus Shakeshaft's original Sturmian results are largely *numerically* correct.

Are these results converged within the s,p manifold? This can be answered by referring to Table II, in which the present results with a basis $\leq 16(s,p)$ on each proton (92 states in all) are compared with the just-noted 24-state results of Shakeshaft. The cross sections have been obtained using a stringent set of parameters, and the error in unitarity is again small [36]. The present cross sections with $n_{\max}=16$ may be converged within about 1% with respect to increasing $n_{\max}$: at the tested energies 15(10)45 keV, values with $n_{\max}=17$ differ by $\leq 1\%$ from those with $n_{\max}=16$, except for a 3% difference for $2s$ excitation at 45 keV. The variation in each cross section with increasing $n_{\max}$ is typically a damped oscillation. (The CPU time increases very rapidly with $n_{\max}$ for large $n_{\max}$, e.g., by about a factor of 7 on increasing $n_{\max}$ from 16 to 17 at these four energies.) Except for $1s,2s$ capture, differences from Shakeshaft's 24-Sturmian results are seen to be significant, particularly for $2s,2p_0,2p_1$

TABLE II. Coupled-Sturmian cross sections (10^{-17} cm^2) for excitation and electron transfer in p-H collisions using the basis $\leq(16s,16p)$ on each proton (92 states in all). Numbers in parentheses are percent differences from Shakeshaft's 24-Sturmian results.

E	Excitation			Transfer			
(keV)	$2s$	$2p_o$	$2p_1$	$1s$	$2s$	$2p_o$	$2p_1$
15	0.840(−13)	0.896(−32)	1.52(−4)	58.0(1)	3.50(3)	0.890(−29)	2.17(12)
20	1.29(−32)	1.40(−24)	2.09(27)	42.0(1)	4.20(<1)	0.854(−11)	1.48(17)
25	1.61(−28)	1.88(−6)	2.73(33)	30.4(1)	4.13(−2)	0.733(3)	1.00(19)
35	1.81(4)	2.62(30)	3.78(8)	16.3(2)	2.98(−4)	0.486(8)	0.483(14)
40	1.84(29)	2.91(26)	4.12(−1)	12.2(3)	2.38(−4)	0.385(6)	0.344(10)
45	1.85(44)	3.06(11)	4.37(−6)	9.21(4)	1.89(−3)	0.304(5)	0.249(6)
55	1.68(13)	3.05(−18)	4.75(−4)	5.44(5)	1.18(<1)	0.189(8)	0.138(4)
60	1.52(−9)	3.01(−23)	4.91(<1)	4.25(5)	0.937(2)	0.147(8)	0.105(6)
70	1.27(−28)	3.11(−17)	5.12(6)	2.67(5)	0.581(1)	0.0880(6)	0.0634(10)
125	0.887(9)	2.57(−1)	4.59(−6)	0.336(1)	0.0704(4)	0.0116(24)	0.0059(7)

TABLE III. Cross sections (in units of 10^{-17} cm^2) for electron transfer to excited states of H (upper half) and for ionization and direct excitation (lower half) in p-H collisions using the Sturmian basis $\leq 16(s,p,d)$ on each center (176 states in all). Numbers in parentheses are *absolute* differences in the last digit(s) from the cross sections of Shakeshaft [8] using a scaled-Sturmian basis $\leq 9s,8p,6d$ on each center (70 states in all).

E (keV)	$1s$	$2s$	$3s$	$2p$	$3p$	$3d$	
15	58.35(0)	3.41(0)	0.50(−3)	3.11(1)	0.63(−11)	0.17(−3)	
25	30.51(16)	4.00(2)	0.94(1)	1.75(1)	0.54(2)	0.06(0)	
50	6.98(20)	1.41(2)	0.43(−2)	0.37(−3)	0.12(−2)	0.01(−1)	
75	2.11(1)	0.44(2)	0.14(0)	0.10(1)	0.03(0)	0.003(−1)	
E (keV)	Ioniz.	$2s$	$3s$	$2p$	$3p$	$3d$	H-α
15	4.0(9)	0.88(0)	0.17(−1)	2.52(6)	0.42(−5)	0.18(−3)	0.39(−6)
25	10.0(15)	1.64(8)	0.34(−10)	4.84(−1)	0.74(−12)	0.29(−5)	0.71(−17)
50	17.3(14)	1.7(−1)	0.3(−1)	7.5(6)	1.3(−1)	0.3(−2)	0.8(−3)
75	16.2(12)	1.3(1)	0.3(0)	8.1(1)	1.2(0)	0.2(0)	0.7(0)

excitation—as much as 30–40 %. The differences oscillate with energy over the tabulated energy range and may be regarded as error estimates for the smaller-basis results. The smaller-basis $2s$ excitation cross section has a spurious dip at 45 keV, whereas the larger-basis cross section has a peak there, consistent with experimental results to be presented in Sec. III.

2. Symmetric s,p,d basis

Cross sections for electron transfer, excitation, and ionization in 15–75 keV p-H collisions are given in Table III using the Sturmian basis $\leq 16(s,p,d)$ on each center (176 states in all) and compared with the cross sections of Shakeshaft [8] using a scaled-Sturmian basis $\leq 9s,8p,6d$ on each center (70 states in all). There is, for the most part, little disagreement

TABLE IV. Coupled-Sturmian cross sections (in units of 10^{-17} cm^2) for electron transfer to excited states of H (upper half) and for ionization and direct excitation (lower half) in p-H collisions using the basis $\leq 16(s,p,d)$ on each center (176 states in all). Numbers in parentheses are the differences in the last digit from values obtained with the basis $\leq 13(s,p,d)$ on each center (140 states in all).

E (keV)	$1s$	$2s$	$3s$	$2p$	$3p$	$3d$	All	
1	170.7(1)	0.047(0)	0.002(0)	2.270(0)	0.021(0)	0.020(0)	173.0(0)	
1.563	153.1(0)	0.080(−1)	0.003(−1)	2.631(0)	0.054(1)	0.051(0)	155.9(0)	
3	127.5(−1)	0.281(1)	0.004(−1)	2.898(1)	0.129(1)	0.107(−2)	131.0(0)	
4	114.5(0)	0.449(1)	0.006(−1)	2.691(−1)	0.169(1)	0.200(0)	118.1(0)	
5.16	103.4(0)	0.682(2)	0.016(0)	2.725(3)	0.215(−2)	0.258(1)	107.5(0)	
8	87.63(−1)	1.53(0)	0.08(−1)	3.21(−1)	0.33(−1)	0.31(0)	93.60(−1)	
15	58.35(0)	3.41(0)	0.50(−2)	3.11(0)	0.63(−3)	0.17(0)	67.41(−1)	
25	30.51(3)	4.00(0)	0.94(−5)	1.75(0)	0.54(0)	0.06(0)	39.45(−4)	
50	6.98(2)	1.41(−1)	0.43(−3)	0.37(−1)	0.12(−1)	0.01(0)	10.04(−1)	
75	2.11(1)	0.44(0)	0.14(−1)	0.10(0)	0.03(0)	0.003(0)	3.05(2)	
100	0.78(1)	0.16(1)	0.05(0)	0.03(0)	0.01(0)	0.001(0)	1.11(1)	
E (keV)	Ioniz.	$2s$	$3s$	$2p$	$3p$	$3d$	All	H-α
1	0.004(−1)	0.047(0)	0.002(0)	2.264(0)	0.021(0)	0.020(0)	2.359(−1)	0.025(0)
1.563	0.015(−1)	0.087(0)	0.003(0)	2.631(0)	0.054(1)	0.050(0)	2.843(1)	0.059(0)
3	0.095(−5)	0.350(−1)	0.009(−1)	3.064(−1)	0.139(1)	0.091(−1)	3.733(2)	0.116(−2)
4	0.205(−11)	0.509(1)	0.012(−1)	3.295(−1)	0.153(2)	0.223(0)	4.309(6)	0.253(−1)
5.16	0.35(0)	0.601(0)	0.027(1)	3.104(0)	0.217(−3)	0.294(3)	4.49(1)	0.347(3)
8	1.07(1)	0.48(0)	0.08(0)	2.24(−1)	0.34(1)	0.22(1)	3.88(0)	0.33(0)
15	3.97(3)	0.88(0)	0.17(0)	2.52(0)	0.42(1)	0.18(0)	4.88(−1)	0.39(−1)
25	10.03(6)	1.64(0)	0.34(−1)	4.84(2)	0.74(1)	0.29(0)	9.19(−2)	0.71(−2)
50	17.3(−2)	1.7(−1)	0.3(0)	7.5(−3)	1.3(1)	0.3(0)	13.0(−1)	0.8(0)
75	16.2(2)	1.3(0)	0.3(0)	8.1(7)	1.2(0)	0.2(0)	12.9(4)	0.7(0)
100	13.7(4)	1.1(1)	0.2(0)	7.2(−1)	1.4(1)	0.2(0)	11.8(3)	0.7(1)

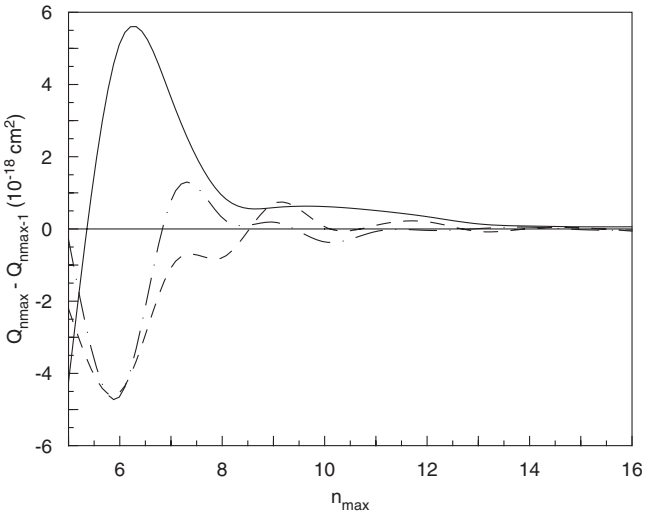

FIG. 2. Successive differences between cross sections for electron transfer in 25 keV p-H collisions with the two-center symmetric Sturmian bases $\leq n_{\max}(s,p,d)$ and $\leq(n_{\max}-1)(s,p,d)$. Solid curve, transfer to $1s$; dashed curve, transfer to $2s$; dashed-dotted curve, transfer to $2p$. A smooth curve has been drawn between values for different $n_{\max}$.

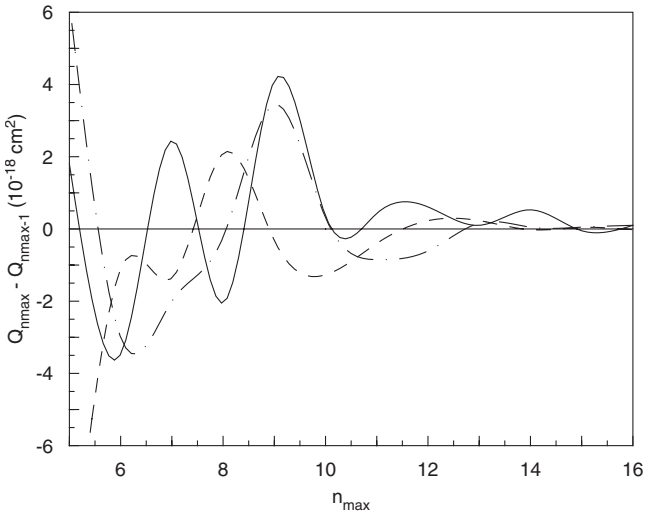

FIG. 3. Successive differences between cross sections for ionization and direct excitation in 25 keV p-H collisions with the two-center symmetric Sturmian bases $\leq n_{\max}(s,p,d)$ and $\leq(n_{\max}-1)(s,p,d)$. Solid curve, ionization; dashed curve, direct excitation to $2s$; dashed-dotted curve, direct excitation to $2p$.

between the present and Shakeshaft's s,p,d-basis cross sections for capture or excitation to states up to $n=2$ (none exceeding 8% when the difference in the last digit exceeds 1 unit), but there are some significant disagreements for ionization and for capture or excitation to $n=3$ states—as much as 30%—probably reflecting incomplete basis convergence of Shakeshaft's calculation within the s,p,d manifold.

C. Additional convergence tests

1. Symmetric s,p,d basis

A more thorough test of convergence of the present Sturmian cross sections within the s,p,d manifold is given in Table IV. Shown are absolute differences of cross sections using the same s,p,d Sturmian basis as in the preceding section [$\leq 16(s,p,d)$ on each center (176 states in all)] from values obtained with the basis $\leq 13(s,p,d)$ on each center (140 states) [37]. Usually, the absolute sensitivity of the cross sections to increasing $n_{\max}$ from 13 to 16 does not exceed 1 unit in the last tabulated digit. For those cross sections whose absolute sensitivities do exceed 1 unit, few have relative sensitivities of at least 5%: $2p$ excitation at 75 keV (9%), $3s$ capture at 25–50 keV (5–6 %), and ionization at 3–4 keV (5%)—most at the higher energies.

These two comparisons with the 176-Sturmian results show that the 140-Sturmian values are substantially more converged than Shakeshaft's 70-scaled-Sturmian values, all within the s,p,d manifold. The 176-Sturmian cross sections are themselves presumably even more converged with respect to increasing the maximum "principal quantum number" $n_{\max}$ of the Sturmians.

To gain perspective on this convergence, successive differences have been plotted in Fig. 2 between cross sections for electron transfer in 25 keV p-H collisions with the two-center symmetric Sturmian bases $\leq n_{\max}(s,p,d)$ and $\leq(n_{\max}-1)(s,p,d)$; corresponding curves for ionization and direct excitation are plotted in Fig. 3. It is seen that the curves are irregularly damped oscillations, significantly so at least up to $n_{\max}\approx 10$, particularly for ionization and direct excitation. Curves for higher transitions (not shown) are also damped oscillations, but of somewhat longer range. Damping at lower energies (not shown) is more rapid and, at higher energies, less so. Thus, it is not surprising that one may need in excess of 100 s,p,d Sturmians (50 on each center) for the cross sections to be moderately converged.

2. Symmetric s,p,d,f basis

The preceding tests have focused first on the numerical accuracy and second on the convergence with respect to increasing the maximum principal quantum number $n_{\max}$ of the Sturmians. It remains to consider the convergence with respect to increasing the maximum angular momentum quantum number $\ell_{\max}$. For this purpose, coupled-Sturmian cross sections for electron transfer, excitation, and ionization in 1–100 keV p-H collisions are given in Table V using the basis $\leq 13(s,p,d,f)$ on each center (220 states in all), together with differences in the last digit(s) from values using the reference 140-state s,p,d basis in the preceding section [$\leq 13(s,p,d)$ on each center]. (The parameters are as for 140 and 176 states.) In most cases, the absolute sensitivity of the cross sections to increasing $\ell_{\max}$ does not exceed 1 unit in the last tabulated digit. For absolute sensitivities that do exceed 1 unit in the last digit, those with relative sensitivities at least 5% are as follows: $3p$ capture or excitation at 1–8 keV ($\leq$25%), $3d$ capture or excitation at 2–3 keV (8–18 %), $3s$ excitation at 5 keV (7%), Balmer-alpha excitation at 2–3 keV (6–14 %), and ionization at 8–15 keV (5–9 %). For these exceptional cases, the greater sensitivity is at the *lower* energies. Thus, the basis $\leq 13(s,p,d,f)$ on each center may be

TABLE V. Coupled-Sturmian cross sections (in units of 10^{-17} cm^2) for electron transfer to excited states of H (upper half) and for ionization and direct excitation (lower half) in p-H collisions using the basis $\leq 13(s,p,d,f)$ on each center (220 states in all). Numbers in parentheses are differences in the last digit(s) from values using the basis $\leq 13(s,p,d)$ on each center (140 states in all).

E (keV)	$1s$	$2s$	$3s$	$2p$	$3p$	$3d$	All
1	170.7(1)	0.048(1)	0.002(0)	2.262(−8)	0.026(5)	0.020(0)	173.1(1)
1.563	153.1(0)	0.080(−1)	0.004(0)	2.616(−15)	0.047(−6)	0.062(11)	156.0(1)
3	127.6(0)	0.278(−2)	0.005(0)	2.861(−36)	0.123(−5)	0.120(11)	131.1(1)
4	114.5(0)	0.445(−3)	0.007(0)	2.647(−45)	0.141(−27)	0.206(6)	118.1(0)
5.16	103.4(0)	0.676(−4)	0.015(−1)	2.677(−45)	0.180(−37)	0.254(−3)	107.5(0)
8	87.64(0)	1.53(0)	0.08(−1)	3.17(−5)	0.30(−4)	0.30(−1)	93.58(−3)
15	58.35(0)	3.39(−2)	0.52(0)	3.09(−2)	0.63(−3)	0.17(0)	67.32(−10)
25	30.48(0)	3.97(−3)	0.98(−1)	1.73(−2)	0.54(0)	0.07(1)	39.42(−7)
50	6.94(−2)	1.42(0)	0.46(0)	0.37(−1)	0.13(0)	0.01(0)	10.03(−2)
75	2.10(0)	0.44(0)	0.15(0)	0.09(−1)	0.03(0)	0.002(−1)	3.03(0)
100	0.78(1)	0.15(0)	0.05(0)	0.03(0)	0.01(0)	0.001(0)	1.11(1)

E (keV)	Ioniz.	$2s$	$3s$	$2p$	$3p$	$3d$	All	H-α
1	0.004(−1)	0.048(1)	0.002(0)	2.255(−9)	0.026(5)	0.020(0)	2.359(−1)	0.026(1)
1.563	0.015(−1)	0.087(0)	0.003(0)	2.618(−13)	0.047(−6)	0.061(11)	2.844(2)	0.069(10)
3	0.102(2)	0.345(−6)	0.010(0)	3.023(−42)	0.135(−3)	0.099(7)	3.725(−6)	0.125(7)
4	0.218(2)	0.500(−8)	0.014(1)	3.251(−45)	0.128(−23)	0.225(2)	4.306(3)	0.254(0)
5.16	0.36(1)	0.592(−9)	0.028(2)	3.063(−41)	0.176(−44)	0.296(5)	4.48(0)	0.345(1)
8	1.16(10)	0.48(0)	0.08(0)	2.21(−4)	0.29(−4)	0.22(1)	3.83(−5)	0.34(1)
15	4.15(21)	0.88(0)	0.17(0)	2.49(−3)	0.40(−1)	0.17(−1)	4.86(−3)	0.39(−1)
25	10.26(29)	1.63(−1)	0.34(−1)	4.78(−4)	0.72(−1)	0.29(0)	9.16(−5)	0.72(−1)
50	17.7(2)	1.7(−1)	0.3(0)	7.7(−1)	1.2(0)	0.3(0)	13.0(−1)	0.8(0)
75	16.1(1)	1.3(0)	0.3(0)	7.5(1)	1.2(0)	0.2(0)	12.4(−1)	0.7(0)
100	13.4(1)	1.0(0)	0.2(0)	7.4(1)	1.3(0)	0.2(0)	11.6(1)	0.6(0)

more reliable for 1–15 keV than the basis neglecting f Sturmians.

3. Asymmetric s,p,d,f basis

The preceding bases are symmetric—that is, with the same Sturmians centered on both the projectile and the target nuclei. Whether they are overly complete depends on the accuracy with which the calculations are carried out, which is believed to be adequate in the present calculations. However, it is clear that the symmetric bases cannot be enlarged much further in the present scheme for two reasons: first, at low energies of about 1 keV, the calculations take a long time; see Fig. 4. (These computing times are on a 3.3 GHz IBM ThinkPad. They increase with decreasing energy with the 176- and the 220-Sturmian bases at energies of about 10 keV or less (and with the 281-Sturmian basis over its entire energy range), attributable to the smaller z-step size required, owing to the more rapidly varying energy phase. On the other hand, the computing time generally levels off or increases with *increasing* energy from 10 to 100 keV, qualitatively owing to the increasing number of points N_λ and, to a lesser extent, N_μ needed in evaluating the charge-exchange matrix elements [10].)

Second, at higher intermediate energies of at least about 100 keV, the convergence with respect to increasing the size of the symmetric basis (monitored by $n_{\max}$) is slow. An alternate procedure at the higher energies is to use a very asym-

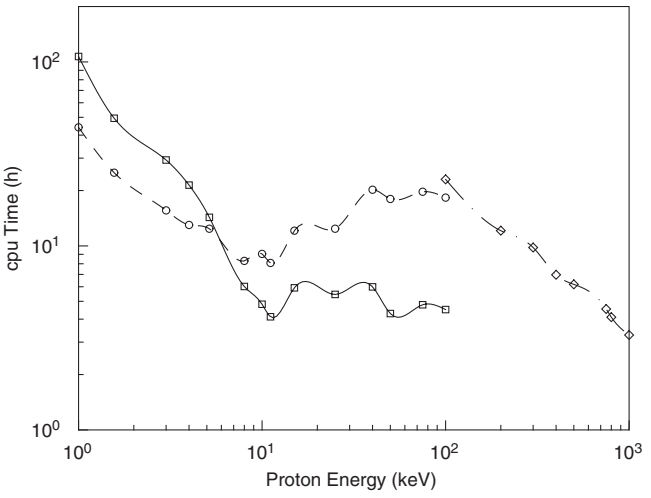

FIG. 4. Computing time to determine cross sections using three production Sturmian bases: circles, 176 Sturmians; squares, 220 Sturmians; diamonds, 281 Sturmian.

TABLE VI. Coupled-Sturmian cross sections (in units of 10^{-18} cm^2) for direct excitation in p-H collisions using the basis $\leq 30(s,p,d,f)$ on the target and $1s$ on the projectile (281 states). Numbers in parentheses are differences in the last digit(s) from values with a 280-state single-center basis.

E (keV)	$2s$	$3s$	$4s$	$2p$	$3p$	$4p$	$3d$	$4d$	$4f$
100	10.48(29)	2.32(9)	0.906(37)	77.6(4)	13.2(1)	4.66(6)	1.85(−4)	0.890(−21)	0.037(−1)
200	5.21(2)	1.094(6)	0.418(3)	58.3(0)	9.92(0)	3.51(0)	0.862(−5)	0.412(−3)	0.0107(−1)
300	3.42(0)	0.704(0)	0.266(0)	46.3(0)	7.85(−1)	2.78(0)	0.547(−1)	0.260(−1)	0.0055(0)
400	2.54(0)	0.518(0)	0.195(0)	38.6(0)	6.52(−1)	2.31(0)	0.398(−1)	0.189(0)	0.0036(0)
500	2.02(0)	0.409(0)	0.153(0)	33.2(0)	5.60(−1)	1.98(0)	0.313(0)	0.149(0)	0.0027(0)
750	1.33(0)	0.268(0)	0.100(0)	24.9(0)	4.19(0)	1.48(0)	0.204(0)	0.0968(0)	0.0016(0)
1000	0.993(0)	0.199(0)	0.0741(0)	20.2(0)	3.38(0)	1.19(0)	0.151(0)	0.0718(0)	0.0012(0)

metric basis of functions centered almost entirely on the target—an appropriate procedure because at these energies direct excitation and ionization dominate electron transfer. This procedure was used by the author on other systems [10], following Ford *et al.* [17].

Accordingly, as given in Table VI, coupled-Sturmian cross sections have been calculated for direct excitation in 100–1000 keV p-H collisions using the basis $\leq 30(s,p,d,f)$ on the target and only $1s$ on the projectile (281 states). (The unitarity check again suggests that, with the parameters chosen here [38], the cross sections are numerically accurate to the tabulated digits.) Calculations have also been carried out with the basis $\leq 25(s,p,d,f)$ on the target and $1s$ on the projectile basis (231 states). Except for the $4s$ state, differences between the 231- and the 281-state results do not exceed 1 unit in the third digit at any energy, and at the higher energies differences are generally in at worst the fourth digit; for $4s$, the difference between the 231- and the 281-state results is 1% at all energies.

Also shown in Table VI are differences in the last digit(s) from values with a 281-state basis as above, but neglecting the $1s$ state centered on the projectile, i.e., a 280-state single-center basis. At energies of at least 300 keV, these differences are at most 1 unit in the last digit, and only at the lowest energy (100 keV) do they exceed 1% for some states. The single-center results will be compared in Sec. III with those of Ford *et al.* using another large single-center basis. Note that with the present large asymmetric basis it has been possible to extract excitation cross sections through $n=4$.

Tests of sensitivity of the asymmetric cross section to increasing $\ell_{\max}$ further have been carried out: Coupled-Sturmian cross sections have been determined for direct excitation in 100–1000 keV p-H collisions using the basis $\leq 12(s,p,d,f,g)$ on the target and $1s$ on the projectile (141 states). [The test has been extended to 1–16 MeV using the basis $\leq 15(s,p,d,f,g)$ on the target only (185 states).] Through excited states up to $4f$, the effect of including g states is at most 1 unit in the third digit, except for $4d$ at 100 keV (a 1% change) and $4f$ at the lower energies ($\leq 10\%$ changes) [39].

D. Summary of results

The coupled-Sturmian results are those obtained with the two symmetric production bases (1) $\leq 16(s,p,d)$ and (2) $\leq 13(s,p,d,f)$ on each center (respectively, 176 and 220 states in all) over the energy range of 1–100 keV given in Tables IV and V, respectively, which may be joined with results in Table VI using (3) the asymmetric basis $\leq 30(s,p,d,f)$ on the target and $1s$ on the projectile (281 states) at the energies of 100–1000 keV. [For excitation and ionization, these results will be extended to 16 MeV using the one-center basis $\leq 30(s,p,d,f)$ and compared with first Born results in Sec. III B 3.]

Few absolute differences between the 176- and the 220-state cross sections exceed 1 unit in the last digits of Tables IV and V. When they do, only the following cross sections differ by more than 5%: some smaller $n=3$ excitation or transfer cross sections at 1–8 keV ($\leq 20\%$), $3s$ transfer at 50 keV (6%), $2p$ or $3p$ excitation at 75–100 keV ($\leq 9\%$), and ionization at 3–8 keV ($\leq 8\%$). For the most part, at least up to 15 keV, the 220-state cross sections are probably the more reliable. An exception may be the 176-state $3s$ excitation and transfer cross sections, which may be more reliable than the 220-state values at all energies, owing to the better representation of the $3s$ state (with 16 rather than 13 Sturmians).

For direct excitation to individual states up to $3d$, these symmetric 176- or 220-state cross sections for 1–100 keV may be compared at the overlapping energy of 100 keV with the asymmetric 281-state cross sections given in Table VI for 100–1000 keV. The 220- and the 281-state cross sections agree to within the fewer digits tabulated for the 220-state values, except for $2p$ (for which the agreement is still to within 5%).

The individual-state coupled-Sturmian cross sections for electron transfer and direct excitation are shown in Fig. 5 for 1–100 keV p-H collisions using the symmetric 176-Sturmian basis. Note that the capture and the excitation curves for a given $n\ell$ merge on the left. They split for each $n\ell$ as the energy is increased, with the excitation curve being higher on the right than the capture curve.

The cross sections for electron transfer are graphed separately from the excitation curves in Fig. 6, now with the 220-state basis as well as the 176-state basis. Note that on the scale of the graph it is hard to distinguish the results with the two bases. The lowest two curves are error estimates: the absolute difference of the summed cross section (including all channels) from $\pi\rho_{\max}^2$ with either basis. Only for $3s$ capture at the lower energies and $3p,3d$ capture at the higher

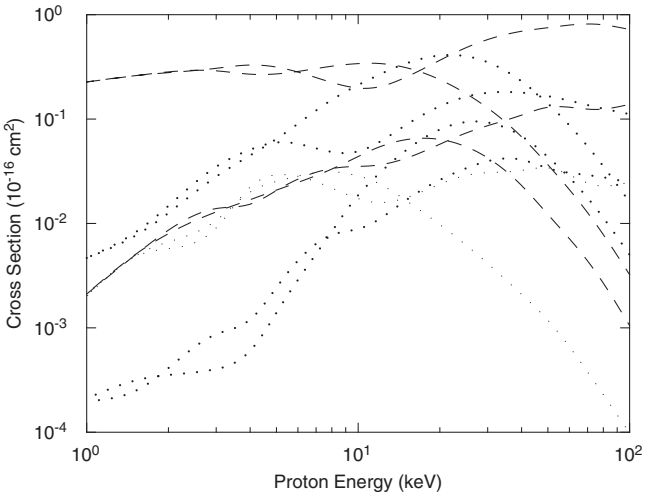

FIG. 5. Coupled-Sturmian cross sections for electron transfer and direct excitation in p-H collisions using the symmetric 176-Sturmian basis. The capture and the excitation curves for a given $n\ell$ merge on the left; from top to bottom on the left they are for $2p$, $2s$, $3p$ and $3d$ (faint dotted curves), and $3s$. Each excitation curve on the right is higher than the capture curve of the same $n\ell$.

energies is the error estimate at all comparable to the cross section.

The cross sections for direct excitation in p-H collisions are graphed in Fig. 7 with the 176-state basis (extended to higher energies with the 281-state basis), as well as the 220-state basis. Again, it is difficult to distinguish the results with the 176- and the 220-state bases. The error estimates are substantially less than the individual cross sections, except possibly for $3s$ at low energies.

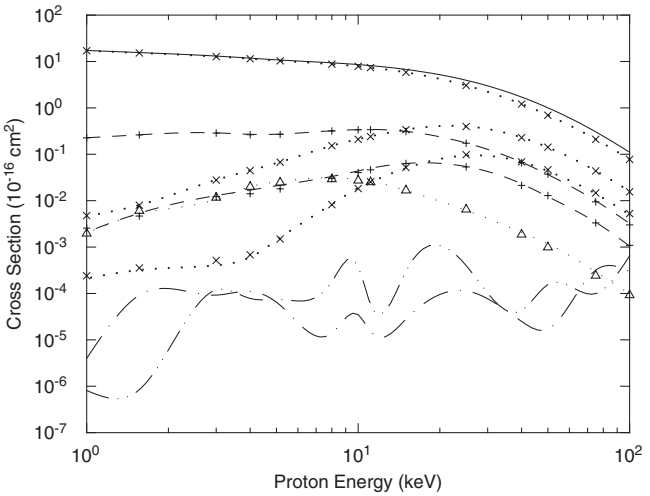

FIG. 6. Coupled-Sturmian cross sections for electron transfer in p-H collisions. The upper curves from top to bottom on the left are for capture to all states (solid curve) and to the $1s$, $2p$, $2s$, $3p$ and $3d$ (faint dotted curve), and $3s$ states using a 176-Sturmian basis. The symbols (triangles for $3d$) are corresponding individual-state values with the 220-state basis. The lowest two (dashed-dotted) curves are unitarity error estimates with the two bases.

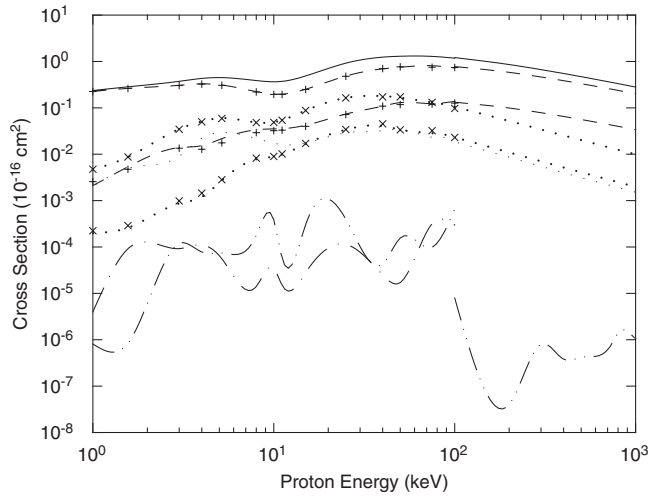

FIG. 7. Coupled-Sturmian cross sections for direct excitation in p-H collisions. The upper curves from top to bottom on the left are for direct excitation to all available excited states (solid curve) and to the $2p$, $2s$, $3p$ and $3d$ (faint dotted curve), and $3s$ states using a 176-Sturmian basis, joined at 100 keV to higher-energy curves with the 281-Sturmian basis. The symbols (for clarity omitted for $3d$) are individual-state values with the 220-Sturmian basis. The lowest (dashed-dotted) curves are error estimates.

III. COMPARISON WITH EXPERIMENTAL AND OTHER THEORETICAL RESULTS

A. Low and intermediate energies

Consider first results mainly at intermediate energies up to 50 or 100 keV. The various electron-transfer cross sections peak below 50 keV, and the structure in these and the direct-excitation cross sections is confined to this range.

1. Electron transfer to all states

Shown in Table VII are coupled-state cross sections for electron transfer to all states and to the $2p$ and the $2s$ states in intermediate-energy p-H collisions. The total electron transfer is by far the largest and, therefore, the least sensitive of these three cross sections to approximations. It is seen that the total cross sections with the three-center-atomic and the relatively small two-center-atomic-plus-pseudostate bases agree fairly closely (within 6%) from 1.563 to 15 keV with the two coupled-Sturmian cross sections (which themselves are virtually identical); the agreement for the purely atomic-state basis is almost as good (within 8%). Even at 25 and 50 keV, the atomic-plus-pseudostate and the atomic-state cross sections agree to at worst 13% with the Sturmian cross section. The resonant process is clearly well represented by just a few coupled atomic states. On the other hand, the large-basis Hylleraas cross section only agrees to within 15% over the energy range of 1.563–15 keV. At 50 keV, the Hylleraas cross section differs by 50%, probably because the Hylleraas basis lacks translational factors, which should be important there. Because of this disagreement even for total transfer, the Hylleraas results for excited states will not be considered here; they were included in the recent review paper by the author [25], along with some other results omitted here.

TABLE VII. Coupled-state cross sections (in units of 10^{-17} cm^2) for electron transfer to all states and the $2p$ and the $2s$ states of H in p-H collisions at various intermediate proton energies E (respectively, the upper, the middle, and the lower sections of the table).

			E (keV)						
Type of basis	Number of functions	Author	1.563	3	5.16	8	15	25	50
3-c atomic	28 or 36	Winter and Lin [21]	152	129	105	90.2	63.1		
2-c Sturmian	176	Winter (present)	156	131	108	93.6	67.4	39.5	10.0
2-c Sturmian	220	Winter (present)	156	131	108	93.6	67.3	39.4	10.0
2-c atomic+pseudo	14	Cheshire *et al.* [3]	165[a]	130[a]	105[a]	90[a]	63.3	34.6	9.0[a]
2-c atomic	8	Cheshire *et al.* [3]	155[a]	125[a]	105[a]	90[a]	61.8	34.4	8.9[a]
Hylleraas	mixed	Lüdde and Dreizler [40]	133[a]	116[a]	94[a]	85.3	63[a]	37.1	5.1
Molecular, opt. factors	10	Kimura and Thorson [18]	2.3[a]	2.9[a]	3.7[a]	4.1[a]			
Molecular, opt. factors	362	Zou *et al.* [19]	2.0[a]	2.8[a]	3.7[a]	4.4[a]			
3-c atomic	28–36	Winter and Lin [21]	2.63	2.93	2.51	3.45	2.44		
2-c augm. atomic (AO+)	22	Fritsch and Lin [42]	2.66	2.92	2.73	3.78	3.39		
2-c atomic+pseudo	40	Fritsch and Lin [43]			3.0[a]	3.4[a]	2.9[a]	1.8[a]	0.48[a]
2-c atomic+pseudo	96	Kuang and Lin [15]					3.1[a]	1.7[a]	0.38[a]
2-c Sturmian	176	Winter (present)	2.63	2.90	2.73	3.21	3.11	1.75	0.37
2-c Sturmian	220	Winter (present)	2.62	2.86	2.68	3.17	3.09	1.73	0.37
2-c atomic+pseudo	14	Cheshire *et al.* [3]	2.5[a]	2.9[a]	3.0[a]	3.3[a]	2.03	1.59	0.59[a]
2-c momentum		Sidky and Lin [44]						1.96	0.447
Molecular, opt. factors	10	Kimura and Thorson [18]	0.12[a]	0.34[a]	0.72[a]				
Molecular, opt. factors	362	Zou *et al.* [19]	0.13[a]	0.32[a]	0.71[a]	1.3[a]			
3-c atomic	28–36	Winter and Lin [21]	0.0833	0.260	0.697	1.07	3.65		
2-c atomic+pseudo	40	Fritsch and Lin [43]				1.4[a]	3.4[a]	4.2[a]	1.4[a]
2-c atomic+pseudo	96	Kuang and Lin [15]					3.5[a]	3.9[a]	1.5[a]
2-c Sturmian	176	Winter (present)	0.080	0.281	0.682	1.53	3.41	4.00	1.41
2-c Sturmian	220	Winter (present)	0.080	0.278	0.676	1.53	3.39	3.97	1.42
2-c momentum		Sidky and Lin [44]						3.99	1.38

[a]Graphically interpolated values.

Shown in Fig. 8 are the experimental results reported by McClure in 1966, with an estimated accuracy of 5%; the omitted error bars are no larger than the graphical circles. Except for the lowest-energy experimental point at about 2 keV, there is an excellent agreement between the graphed theoretical results and this experiment, with the present results offering some improvement over the small-basis results at energies of about 25 keV.

Also shown are the experimental results of Chen *et al.* and Melchert *et al.* for electron transfer in He^{2+}-He^{+} collisions, scaled to p-H collisions using the relation $Q(v,Z)=Q(v/Z,1)/Z^2$ noted in the Introduction for $Z=2$. Only a few of the error bars are given; they are comparable to, or smaller than, the symbols. Chen *et al.* and Melchert *et al.* note additional absolute errors in their data of 7.4% and 9%, respectively (not shown). The agreement is excellent with their data, including that of Melchert *et al.* at higher energies if the absolute errors were included.

2. Electron transfer to the 2p state

Consider second capture to the $2p$ state in Table VII. This is the more likely of the two $n=2$ capture processes over the lower intermediate-energy range. The three-center-atomic and two-center AO+ cross sections differ from (the average of) the two Sturmian cross sections by at most 2% at the two lowest energies, but up to 20% at higher energies. Also shown at higher energies is the 40-atomic-plus-pseudostate cross section of Fritsch and Lin, regarded by them as improving on their AO+ cross section at energies above 15 keV by accounting more fully for the continuum and, indeed, the disagreement with the Sturmian cross sections is not more than about 10%, except for a 30% disagreement at the highest energy of 50 keV. The oscillating disagreement of the 14-atomic-plus-pseudostate cross section with the Sturmian cross sections is up to about 60%. (For the atomic-state cross section [3], not shown, the oscillating disagreement is still more unsatisfactory—up to a factor of 2.)

Toshima [16] reported large-basis results for electron transfer, ionization, and excitation in p-H collisions and tabulated at 1 and 4 keV some of these cross sections with a symmetric two-center 394-Gaussian-pseudostate basis. (His values for $2p$ with a predominantly target-centered basis of the same size agree to better than 3% with his own symmetric-basis results.) The present Sturmian results for $2p$

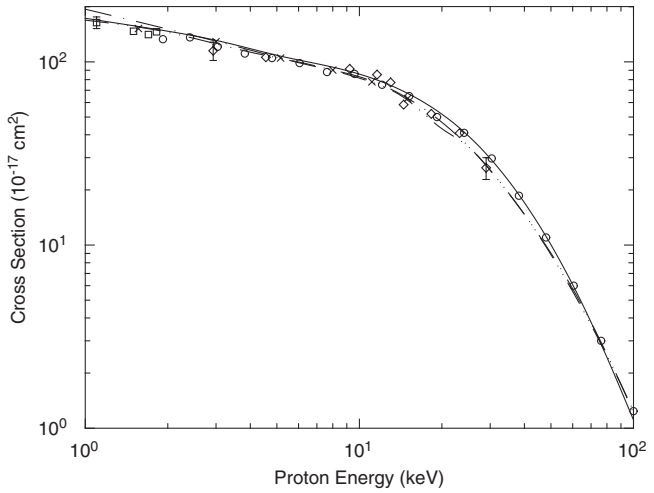

FIG. 8. Cross sections for electron transfer to all states of H in p-H collisions. Coupled-state results: crosses, three-center atomic [21]; solid line, 176 or 220 Sturmians; dashed-dotted line, two-center atomic plus pseudo [3]; dashed-double-dotted line, two-center atomic [3]. Experimental results: circles, McClure [41]; squares, Chen *et al.* [31]; diamonds, Melchert *et al.* [30]. The last two experimental results are for He^{2+}-He^{+} collisions scaled to p-H collisions.

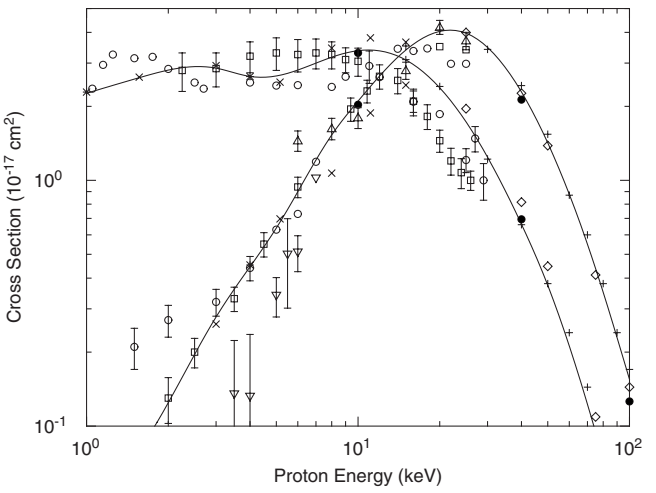

FIG. 9. Cross sections for electron transfer to the $2p$ state (upper curve on the left) and $2s$ state (lower curve on the left) in p-H collisions. Coupled-state results: crosses, three-center atomic [21]; plus signs, two-center 96 atomic plus pseudo [15]; solid line, two-center 220 Sturmians; asterisks (at 1 and 4 keV only), two-center 394 Gaussians [16]; diamonds, two-center momentum [44]. Numerical: solid circles, Kołakowska *et al.* [33]. Experimental results for $2p$: open circles, Kondow *et al.* [46]; squares, Morgan *et al.* [47]. Experimental results for $2s$: open circles, Hill *et al.* [49]; squares, Morgan *et al.* [50]; triangles, Chong and Fite [48]; inverted triangles, Bayfield [45].

transfer agree to at least 2% with Toshima's 394-Gaussian results.

The optimized ten-molecular-state cross section of Kimura and Thorson lies below the Sturmian cross sections by about 12% at the lowest tabulated energy, and above by about 30% at its highest energy (8 keV). The recent optimized 362-molecular-state cross section of Zou *et al.* fails to resolve this discrepancy.

Also shown at energies $\geq$15 keV is the 96-atomic-plus-pseudostate (even-tempered-basis) result of Kuang and Lin. For transfer, their cited basis includes 76 atomic states and pseudostates centered on the projectile and 20 atomic states centered on the target nucleus. (For direct excitation, the placement of basis functions on the two centers is reversed.) There is a close agreement (within 3%) with the Sturmian cross sections.

At the higher energies of 25 and 50 keV, the Sturmian cross sections can also be compared with the relatively recent momentum-space result of Sidky and Lin, on which they placed error bars of $\pm$5%. Surprisingly, the agreement is only within 20%. Not shown are the 40-state three-center results of McLaughlin *et al.* [23], stated by them to agree well with the 36-state three-center results [21] for all processes *except* for $2p$ capture at low energies. Unphysically and in contrast to the present Sturmian and the smaller-basis three-center results, their $2p$ capture cross section deviates markedly from the $2p$ excitation cross section at low energies.

Experimental results of Kondow *et al.* and Morgan *et al.* for $2p$ capture are shown in Fig. 9 along with what are perceived to be the more accurate of the previously tabulated theoretical results (plus the results to be considered later for $2s$). The error bars on the data of Kondow *et al.* (omitted here when not larger than the symbols) are relative errors; there is a systematic error, not shown, which, at energies below 15 keV, is believed to be within the error bars. The error bars on the data of Morgan *et al.* omit a 30% absolute uncertainty. It is seen that the cross section of Kondow *et al.*—but not of Morgan *et al.*—confirms the undulating shape, but not the amplitude, of the Sturmian curve at lower energies. At intermediate energies of about 15 keV or higher, the experimental cross sections generally lie below the Sturmian, the 96-atomic-plus-pseudostate, and the momentum-space results.

3. Electron transfer to the **2***s state*

At the lowest tabulated energy, the $2s$ transfer cross section in Table VII (and Fig. 9) is more than an order of magnitude smaller than the $2p$ cross section—the curves crossing at about 15 keV. The $2s$ cross section should therefore be more sensitive at low energies than the $2p$ cross section, and this is indeed the case: at 1.563 keV, the AO+ and the 14-atomic-plus-pseudostate cross sections [3,42] (not shown) differ from either Sturmian cross section by factors of 1.6 and 3.2, respectively, while the much larger 15 keV cross sections agree within 9%. The oscillating atomic-state cross section [3] (also omitted) differs greatly from the Sturmian cross sections. The large-basis optimized-molecular-state cross section in Table VII disagrees significantly with (the average of) the Sturmian values at both 1.563 and 15 keV (by about 60% and 15%, respectively). The triple-center cross section dips 30% below the common Sturmian value at 8 keV. The present Sturmian results for $2s$ transfer agree to at

TABLE VIII. Coupled-state cross sections (in units of 10^{-18} cm^2) for direct excitation to the $2p$ and the $2s$ states in p-H collisions at various intermediate proton energies E (respectively, the upper and the lower sections of the table).

			E (keV)						
Type of basis	Number of functions	Author	1.563	3	5.16	8	15	25	50
Molecular, opt. factors	362	Zou *et al.* [19]	20[a]	27[a]	36[a]	41[a]			
3-c atomic	28–36	Winter and Lin [21]	26.5	29.7	29.4	24.3	23.0		
2-c atomic+pseudo	40	Fritsch and Lin [43]			31[a]	23[a]	24[a]	46[a]	83[a]
2-c atomic+pseudo	96	Kuang and Lin [15]					21[a]	42[a]	83[a]
2-c Sturmian	176	Winter (present)	26.3	30.6	31.0	22.4	25.2	48.4	75
2-c Sturmian	220	Winter (present)	26.2	30.2	30.6	22.1	24.9	47.8	77
2-c atomic+pseudo	14	Cheshire *et al.* [3]	25[a]	30[a]	37[a]	31[a]	21.2	55.2	126[a]
2-c momentum		Sidky and Lin [44]						51.0	65.9
Molecular, opt. factors	10	Kimura and Thorson [18]	1.2[a]	3.2[a]	6.3[a]				
Molecular, opt. factors	362	Zou *et al.* [19]	1.2[a]	3.2[a]	5.7[a]	5.9[a]			
3-c atomic	28–36	Winter and Lin [21]	0.927	3.41	6.03	3.84	8.80		
2-c atomic+pseudo	40	Fritsch and Lin [43]				5.8[a]	8.1[a]	12[a]	19[a]
2-c atomic+pseudo	96	Kuang and Lin [15]					8.6[a]	14[a]	17[a]
2-c Sturmian	176	Winter (present)	0.87	3.50	6.01	4.8	8.8	16.4	17
2-c Sturmian	220	Winter (present)	0.87	3.45	5.92	4.8	8.8	16.3	17
2-c atomic+pseudo	14	Cheshire *et al.* [3]	2.5[a]	6.1[a]	3.6[a]	2.9[a]	10.6	9.04	21[a]
2-c momentum		Sidky and Lin [44]						14.2	14.6

[a]Graphically interpolated values.

least 2% with the 394-Gaussian results of Toshima [16], which he tabulated at 1 and 4 keV—the same level of agreement noted for $2p$ transfer.

At the higher intermediate energies of 15–50 keV, the 40-atomic-plus-pseudostate, the 96-atomic-plus-pseudostate, and the momentum-space cross sections agree with the Sturmian cross sections to within at least 6%—which is less than half the spread for $2p$ in this energy range, probably because of the inversion of the cross sections at these energies and the likely smaller-basis sensitivity of the larger cross section.

Shown in Fig. 9 at 10, 40, and 100 keV is the $2s$ cross section, as well as $2p$ cross section at 10 and 40 keV, obtained by solving the time-dependent Schrödinger equation numerically on a three-dimensional Cartesian lattice [33]. It is seen that there is a generally good agreement with the other graphed theoretical results—specifically, 2–7 % with the 220-Sturmian cross sections, save for a 20% $2s$ disagreement at 100 keV.

And shown in Fig. 9 are the experimental results of Hill *et al.*, Morgan *et al.*, Chong and Fite, and Bayfield; the error bars are relative errors. An estimated 25–30 % absolute error is omitted from the displayed errors of Hill *et al.* and Bayfield, and an absolute error is also omitted from the errors of Morgan *et al.* The three sets of data extending to low energies disagree there, but are in accord at the higher energies, except for one point at 6 keV; it is the lower-energy data of Morgan *et al.* which favor the displayed theoretical cross sections.

4. Direct excitation to the 2p state

Shown in Table VIII are coupled-state cross sections for direct excitation to the $2p$ and the $2s$ states in intermediate-energy p-H collisions. Consider first the $2p$ cross section, which is the larger of the two over the entire energy range, and presumably the less sensitive. The triple-center cross section agrees well (within 9%) with (the average of) the two Sturmian cross sections over the range up to 15 keV, and especially well at the lower energies. In contrast, the large molecular-state calculation disagrees by up to a factor of 1.8 over its more limited range up to 8 keV. The Sturmian results agree to at least 1% with the 394-Gaussian results of Toshima [16] at the low energies of 1 and 4 keV (not shown here). At higher energies up to 50 keV, the 40- and the 96-atomic-plus-pseudostate and the momentum-space results agree to 6–16 % with the average Sturmian cross section. The smaller 14-atomic-plus-pseudostate result disagrees by up to 66%. Omitted from the table are the atomic-state and AO+ pseudostate values [3,42], each differing by up to about 50% from the Sturmian cross sections.

The experimental results for $2p$ excitation are shown in Fig. 10 along with what are probably the more accurate of the theoretical results (as well as results to be considered for $2s$). There is an excellent agreement among the experimental and almost all the theoretical results (except for an exaggerated dip in the triple-center cross section at 11 keV and except for the momentum-space cross section being about 15% too low at 50 keV).

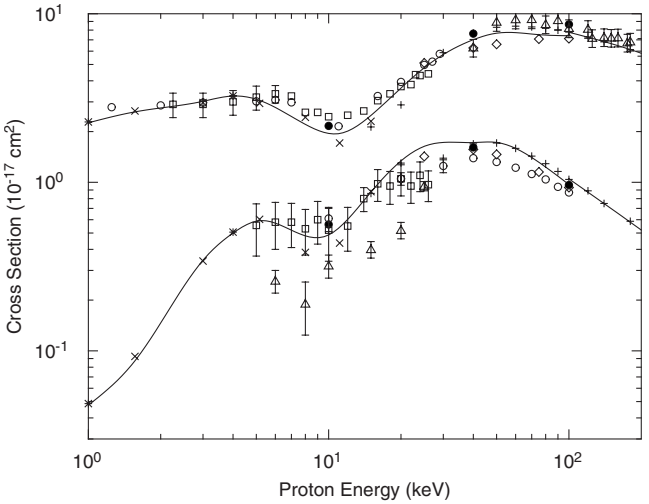

FIG. 10. Cross sections for direct excitation to the $2p$ state (upper curve) and $2s$ state (lower curve) in p-H collisions. The theoretical results are labeled as in Fig. 9, with the addition that the Sturmian curve has been extended beyond 100 keV using the 281-state asymmetric basis. The $2p$ experimental results are labeled as there, with this addition: triangles, Detleffsen *et al.* [52]. The $2s$ experimental results: open circles, Higgins *et al.* [51]; squares, Morgan *et al.* [47]; triangles, Chong and Fite [48].

5. Direct excitation to the 2s state

The $2s$ excitation cross section is much smaller than the $2p$ cross section over the entire energy range displayed in Table VIII, and so should be more sensitive. This is indeed the case: at 1.563 keV, the 10- and the 362-molecular-state cross sections and the omitted AO+ cross section [42] lie above the common Sturmian value by 40–50 %, and for the 362-molecular-state and the AO+ cross sections there are significant disagreements with the Sturmian values at higher energies as well. In contrast, only at the possibly sensitive dip at 8 keV does the triple-center cross section show significant disagreement (20%). The 14-atomic-plus-pseudostate cross section differs from the Sturmian values at all energies; the omitted atomic-state cross section [3] even more so. The present Sturmian results agree to at least 4% with the 394-Gaussian result of Toshima [16] (not shown here), which he tabulated at 1 and 4 keV.

At the higher intermediate energies of 15–50 keV, the 40-atomic-plus-pseudostate cross section agrees with the (average) Sturmian cross section to within only 27%, while the 96-atomic-plus-pseudostate and the momentum-space cross sections agree to within 14% with the Sturmian results.

The experimental $2s$ cross sections are shown in Fig. 10 along with the theoretical cross sections that are considered to be the more accurate. In the range of 5–15 keV there is an excellent agreement of the Sturmian cross section with the experimental values of Morgan *et al.* but not of Chong and Fite; at higher energies most of the theoretical results lie somewhat above the experimental data.

Also shown at 10, 40, and 100 keV are the $2s$ and the $2p$ cross sections obtained numerically [33]. It is seen that there is generally a good agreement with the other theoretical results, as well as with the experimental results. Specifically, there is 6–15 % agreement with the 220-Sturmian cross sections at 10 and 40 keV and with the 281-Sturmian cross sections at 100 keV.

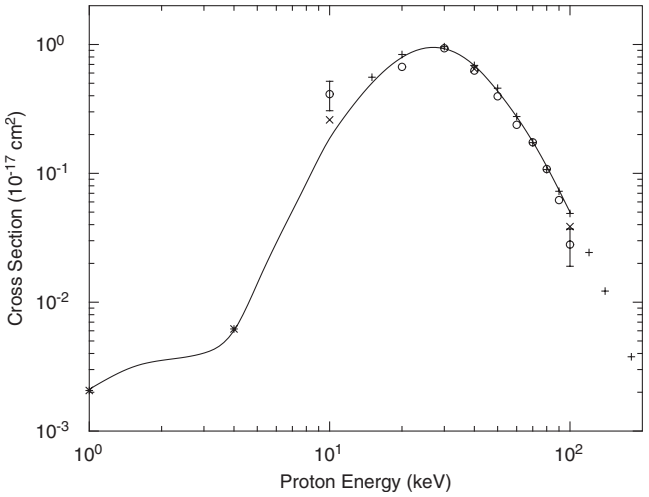

FIG. 11. Cross sections for electron transfer to the $3s$ state of H in p-H collisions. The theoretical results: asterisks (at 1 and 4 keV only), 394 Gaussians [16]; solid line, 176 Sturmians; plus signs, 96 atomic plus pseudo [15]; crosses, numerical (at 10, 40, and 100 keV only) [33]. Experimental results: circles, Hughes *et al.* [53].

6. Electron transfer to the 3s state

Shown in Fig. 11 are the experimental cross sections of Hughes *et al.* for electron transfer to the $3s$ state, along with various theoretical results. The experimental error bars (usually not bigger than the circles) have been omitted at all but the extreme energies (10 and 100 keV), and an absolute error of 17% has also been omitted. Except at the extreme energies, there is an excellent agreement among the displayed theoretical and the experimental results. Note the close agreement between the 176-Sturmian and the 394-Gaussian results at 1 and 4 keV (within 3%). (The 176-Sturmian basis may provide a better representation of the $3s$ state than the 220-Sturmian basis, omitted here, for which the agreement with the Gaussian result is only within 17%.)

7. Direct excitation to the 3p state

Shown in Fig. 12 is the experimental cross section of Detleffsen *et al.* for direct excitation to the $3p$ state, along with theoretical results. The experimental results extend to 800 keV, and so the present Sturmian result has been extended beyond 100 keV by means of the asymmetric 281-state calculation. (Some experimental points below 200 keV have been omitted for clarity.) Both the 176- and the 220-Sturmian results are included up to 100 keV. At lower energies, the 220-Sturmian result is believed to be superior for this state, which is supported by the excellent agreement (within 4%) with the displayed 394-Gaussian results at 1 and 4 keV. There is a dip in the 94-atomic-plus-pseudostate result at 20 keV which is absent in either Sturmian curve there, although the agreement at higher energies is good, as it is with the numerical and the experimental results.

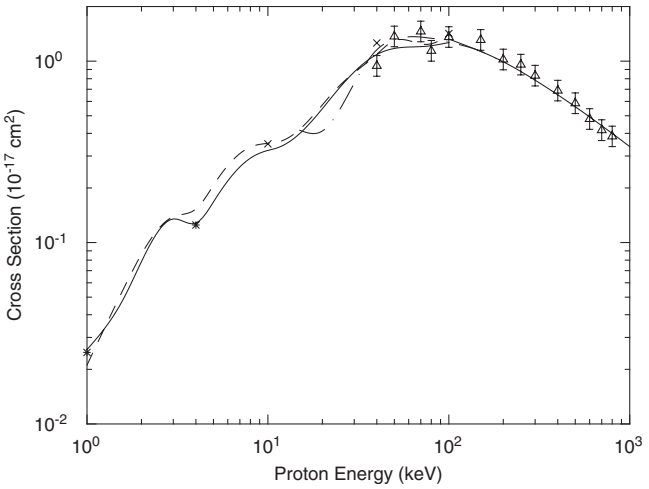

FIG. 12. Cross sections for direct excitation of the $3p$ state of H in p-H collisions. Theoretical results: asterisks (at 1 and 4 keV only), 394 Gaussians [16]; solid line, 220 Sturmians, joined to 281 Sturmians at energies of at least 100 keV; dashed line, 176 Sturmians; dashed-dotted line, two-center 96 atomic plus pseudo [15]; crosses, numerical (at 10, 40, and 100 keV only) [33]. Experimental results: triangles, Detleffsen *et al.* [52].

8. Direct Balmer-alpha ($n=3$) excitation

Shown in Fig. 13 is the 15–100 keV experimental cross section of Donnelly *et al.* for direct Balmer-alpha excitation, which is the sum of the $n=3$ cross sections after first multiplying the otherwise dominant $3p$ cross section by 0.118. Also shown are selected theoretical cross sections over a greater energy range. Note the structure in the 220-Sturmian cross section at lower energies, confirmed by the result with the other Sturmian basis—the two differing significantly only at their highest energy (100 keV), with the 220-state

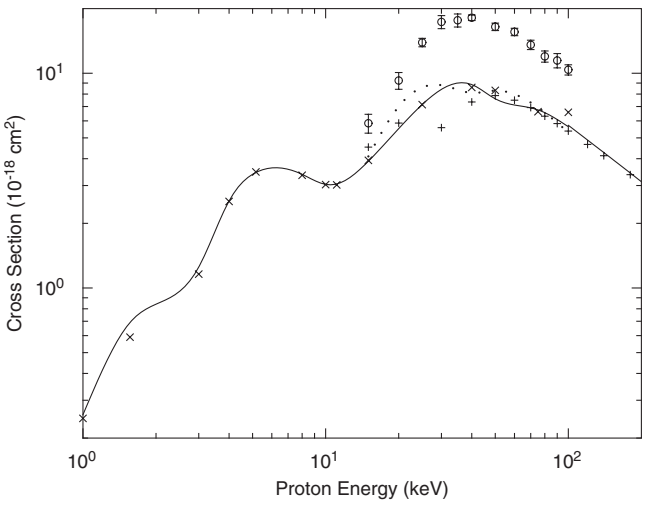

FIG. 13. Cross sections for Balmer-alpha direct excitation in p-H collisions. Theoretical results: solid line, 220 Sturmians, joined to 281 Sturmians at energies of at least 100 keV; crosses, 176 Sturmians; plus signs, 96 atomic plus pseudo [15]; dotted curve, 74 atomic plus pseudo [27]. Experimental results: circles, Donnelly *et al.* [26].

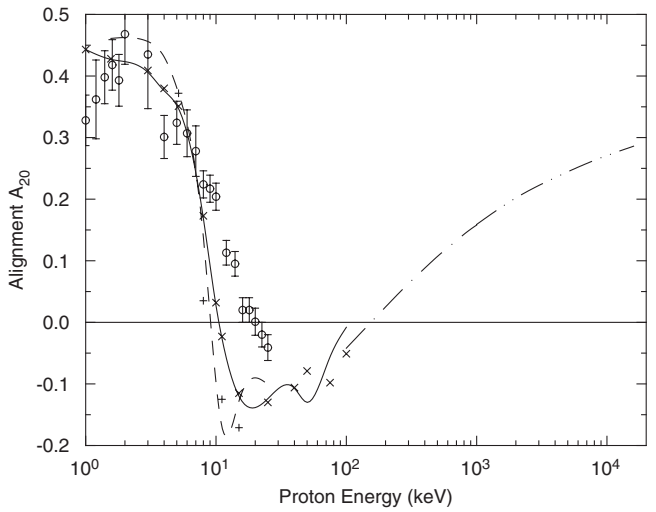

FIG. 14. Integral alignment A_{20} in p-H collisions. Solid curve, 220 Sturmians; crosses, 176 Sturmians; dashed-dotted curve, 281 Sturmians (at 100–1000 keV); plus signs, 36 three-center atomic [55]; dashed curve, 40 three-center atomic [23]; dashed-double-dotted curve, first Born (at 1000–16 000 keV). Experimental results: circles, Hippler *et al.* [54].

result probably being the more reliable there. Except at 30 keV, the 94-atomic-plus-pseudostate cross section also agrees very well. Also shown is a 74-atomic-plus-pseudostate result, which agrees fairly well with the Sturmian result. Not shown is the large-basis single-center result of Ford *et al.* [17] down to 15 keV, which, surprisingly, agrees extremely well with the other theoretical results even at this lower energy. Also omitted is the 40-state triple-center cross section of McLaughlin *et al.* [23], which has an unphysical large oscillation over the energy range of the experiment; this calculation omitted $n=4$ states centered on the nuclei from the basis and may not be converged here.

Not shown with the experimental error bars is a 21% normalization uncertainty and a cascade correction estimated to be at most 15%. These experimental uncertainties are insufficient to bridge the gap between the experimental result and all the displayed theoretical results.

9. Alignment of 2p direct excitation

Shown in Fig. 14 is the experimental integral alignment A_{20} of Hippler *et al.*, defined as the difference between the $2p_1$ and the $2p_o$ cross sections, divided by the total $2p$ excitation cross section. Here, $2p_1$ refers to the $m=1$ or the identical $m=-1$ cross section, *not* to their sum as in Tables I and II. Shown along with the experimental result are 176-, 220-, and 281-Sturmian values, as well as 36- and 40-state three-center values. A positive A_{20} means that $2p_1$ is the larger cross section and a value of 1/2 would imply that the $2p_o$ cross section is negligible. The alignment has a very large uncertainty when the cross sections are nearly equal; the alignment sensitively passes through zero. However, the 176- and the 220-Sturmian alignments are virtually coincident at lower energies and pass through zero *together* on the lower-energy side, differing only from 50 to 100 keV. The 40-state triple-center curve is somewhat higher than the Sturmian

curve at lower energies and passes through zero more rapidly, although it is consistent with the 36-state triple-center cross section. The experimental curve drops off more rapidly than either of the two theoretical curves, but is somewhat closer to the Sturmian curve. At high energies, the 281-Sturmian curve merges smoothly with the Born curve.

10. 3p and 3d transfers and 3s and 3d direct excitations

There do not appear to be any experimental results for these four processes. At 1 and 4 keV, Sturmian results for the other lower excited states were compared in the previous sections with the 394-Gaussian results of Toshima [16], and the agreement was found to be excellent (within 4%, usually even better). For $3s$ excitation, the agreement using the 176-Sturmian basis is to 2% with Toshima's result at 1 keV, but only 18% at 4 keV (at which, however, the agreement is to 0.5% with the 220-Sturmian basis). For $3p$ transfer, $3d$ transfer, and $3d$ excitation at either energy, the agreement with Toshima's results is, as expected, somewhat better using the 220-Sturmian basis (within 4%) than with the 176-Sturmian basis (within about 20% for $3p$ transfer and 5% for $3d$ transfer or excitation).

The 220-Sturmian cross sections for these four processes are also compared with the 94-atomic-plus-pseudostate graphical values of Kuang and Lin [15]. The disagreement at the compared energies of 15, 50, and 100 keV does not exceed three units in the last digit reported in Table V. Only for $3d$ transfer, $3d$ excitation, and $3s$ excitation at 15 keV, and for $3p$ transfer at 50 keV do absolute differences exceed 1 unit in the last digit; for these exceptional cases, the relative differences are 13–19 %. On the other hand, the numerical $3d$ capture and excitation cross sections [33] at 10 and 40 keV are above the 220-Sturmian (as well as 176-Sturmian) values by as much as about 50%.

11. Ionization

Shown in Fig. 15 is the experimental cross section of Shah *et al.* for ionization in p-H collisions. Also shown are coupled-state results: cross sections with 394 Gaussian pseudostates, 96 atomic states and pseudostates, and 220 Sturmians (up to 100 keV, with 281 Sturmians at higher energies). The many-decade graph fails to emphasize some significant discrepancies at the 50 keV peak: the Gaussian and the Sturmian results, which themselves agree within 1% there, lie on average 27% above the experimental curve, whereas the 96-atomic-plus-pseudostate curve agrees closely with experiment (within 2%). The situation is very similar at the highest experimental energy (75 keV): the Gaussian and the Sturmian cross sections agree to 1%, while their average lies 26% above the experimental curve. At both energies, the 176-Sturmian curve (not shown) lies within 2% of the 220-Sturmian curve. The omitted relative experimental uncertainty (well within the circles) and the omitted normalization uncertainty of 5% are insufficient to account for the discrepancy with the Gaussian and the present Sturmian results.

At the low energies of 1 and 4 keV, where the cross section is very small and hence sensitive to numerics, the 220-Sturmian curve (as well as the 176-Sturmian curve, not shown) lies about 20% below the Gaussian points. At least at 1 keV, the extent of agreement is consistent with the estimated accuracy of the present calculations.

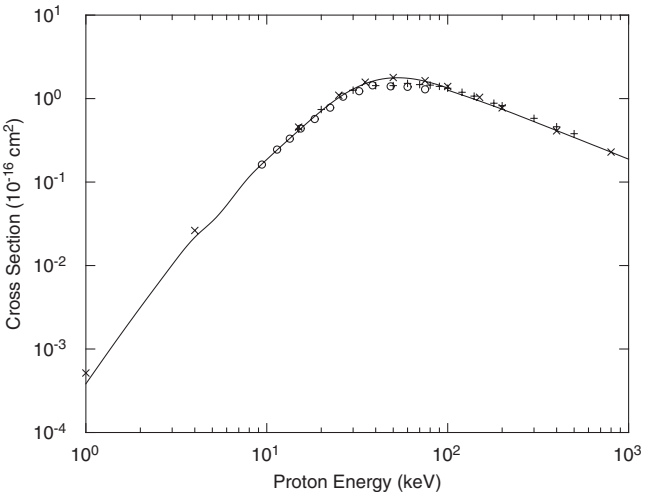

FIG. 15. Cross sections for ionization in p-H collisions. Coupled-state results: crosses, 394 Gaussians [16]; plus signs, 96 atomic plus pseudo [15]; solid line, 220 Sturmians up to 100 keV, joined to 281 Sturmians for higher energies. Experimental result: circles, Shah *et al.* [29].

B. Higher energies

1. Direct excitation

It has been pointed out in Sec. II C 3 that at higher energies an asymmetric basis centered mainly on the target nucleus is appropriate, and results were presented using the Sturmian basis $\leq 30(s,p,d,f)$ on the target and only $1s$ on the projectile (281 states). Cross sections for direct excitation into individual states up to $4f$ were compared in Table VI with those for a single-center basis of 280 states in which the $1s$ state on the projectile was omitted; it was noted that only at the lowest energy (100 keV) do differences exceed 1% for some states. These single-center results are now compared in Table IX with those of Ford *et al.* using a different large single-center basis. At energies of at least 200 keV, absolute differences rarely exceed 1 unit in the last digit, and all relative differences are less than 1%, except for the $4f$ state. Ford *et al.* estimated their cross sections to be accurate to 3%; except for $4f$ at energies up to 300 keV, agreement is indeed to within *at least* 3% or 1 unit in the last digit. Aside from numerical inaccuracy, the only difference between the two calculations should be the inclusion of g,h states by Ford *et al.* However, except for $4d$ at 100 keV and except for $4f$ at energies of 100–400 keV, the effect of g states in the present Sturmian calculation was noted in Sec. II C 3 to be negligible; for these exceptional cases, the inclusion of g states reduces the small discrepancies with those of Ford *et al.* by at least half.

2. Ionization and electron transfer

It was emphasized by Ford *et al.* that with a single-center basis the apparent ionization cross section at higher energies

TABLE IX. Coupled-Sturmian cross sections (in units of 10^{-18} cm^2) for direct excitation in higher-energy p-H collisions using the single-center basis $\leq 30(s,p,d,f)$ on the target (280 states). Numbers in parentheses are differences in the last digit(s) from Ford *et al.* [17] using another large single-center basis.

E (keV)	$2s$	$3s$	$4s$	$2p$	$3p$	$4p$	$3d$	$4d$	$4f$
100	10.19(−1)	2.23(−1)	0.869(−1)	77.2(10)	13.1(2)	4.60(6)	1.89(3)	0.911(19)	0.038(5)
200	5.19(0)	1.088(−2)	0.415(−1)	58.3(4)	9.92(6)	3.51(2)	0.867(−5)	0.415(−1)	0.0108(13)
300	3.42(0)	0.704(−1)	0.266(−1)	46.3(2)	7.86(5)	2.78(1)	0.548(−2)	0.261(−1)	0.0055(5)
400	2.54(0)	0.518(1)	0.195(0)	38.6(1)	6.53(2)	2.31(1)	0.399(−1)	0.189(−1)	0.0036(1)
500	2.02(0)	0.409(1)	0.153(−1)	33.2(1)	5.61(2)	1.98(0)	0.313(−1)	0.149(0)	0.0027(1)
750	1.33(0)	0.268(1)	0.100(0)	24.9(0)	4.19(1)	1.48(1)	0.204(0)	0.0968(1)	0.0016(0)
1000	0.993(2)	0.199(0)	0.0741(0)	20.2(0)	3.38(1)	1.19(0)	0.151(0)	0.0718(1)	0.0012(1)

includes a small but not necessarily negligible electron-transfer component, with the sum of the two processes being termed electron removal. The same statement can be made to a lesser extent about the present cross section with a 281-state basis since, while explicitly including the $1s$ transfer channel, it ignores transfer into excited states, which, if one assumed an n^{-3} rule, would contribute 20% to total transfer.

Shown in Table X are coupled-Sturmian cross sections for ionization, electron removal, and $1s$ capture in 100–800 keV p-H collisions using the basis $\leq 30(s,p,d,f)$ on the target and $1s$ on the projectile (281 states). These results are compared with the cross sections of Toshima for ionization with a symmetric two-center 394-Gaussian basis. It is perhaps surprising that the cross sections differ by $<1\%$ at the two highest energies since the present calculations omit g,h states which, according to the first Born approximation, should contribute $\geq 1\%$ [56]. Also shown are the two-center 94-atomic-plus-pseudostate (even-tempered-basis) results of Kuang and Lin (from their graphs) for ionization and $1s$ capture and the results of Ford *et al.* for electron removal using a large single-center basis. Note that the Sturmian $1s$ capture cross section is the difference between the Sturmian results for electron removal and ionization. For energies ≥ 400 keV, this capture cross section is seen to be $\leq 0.02 \times 10^{-18}$ cm^2; in view of the unitarity check $\Sigma Q \approx \pi \rho_{\max}^2$, it may only be marginally reliable at 800 keV and higher energies. At the lowest energy given here (100 keV), the *symmetric* Sturmian bases may give better results (in Tables IV and V) than the results with the asymmetric basis tabulated here. At this energy, the 176- and the 220-state symmetric bases give 137×10^{-18} and 134×10^{-18} cm^2, respectively, for ionization, and both give 7.8×10^{-18} cm^2 for $1s$ capture; the average of these two ionization cross sections differs by only 2–3 % from the Gaussian and the even-tempered values; and the average Sturmian value for electron removal differs by only 1% from the one-center value. On the other hand, there is a 9% disagreement with the even-tempered value for $1s$ capture at this energy—a disagreement significantly greater than that between the asymmetric-Sturmian and the even-tempered values (1%).

3. Ionization and direct excitation at very high energies: Comparison with the first Born approximation

Shown in Table XI are coupled-Sturmian cross sections for ionization and direct excitation in MeV-energy p-H collisions using the single-center basis $\leq 30(s,p,d,f)$ on the target (280 states) [57,58], together with *percent* differences from results with the first Born approximation. For excitation, doubling the energy about halves the magnitude of the percent difference for each state. These differences exceed 1% for some states up to about 1 MeV; however, by 16 MeV (for which $v/c \approx 0.18$), no difference exceeds 0.1%. For ionization, the approximately constant difference of about 1% between the Born and the Sturmian values at $E \geq 1$ MeV is reduced to about 0.5% using a 380-state Sturmian basis (not

TABLE X. Coupled-Sturmian cross sections (in units of 10^{-18} cm^2) for ionization, electron removal, and $1s$ capture in higher-energy p-H collisions using the asymmetric basis $\leq 30(s,p,d,f)$ on the target and $1s$ on the projectile (281 states). Comparison with the cross sections of Toshima [16] for ionization using a symmetric two-center 394-Gaussian basis; numbers in parentheses are percent differences from the Sturmian values. Also shown are the two-center 94-state even-tempered results of Kuang and Lin [15] for ionization and $1s$ capture, and the results of Ford *et al.* [17] for electron removal using a large single-center basis.

E	Ionization			e^- removal		$1s$ capture	
(keV)	Sturmian	Gaussian	Even tempered	Sturmian	Single center	Sturmian	Even tempered
100	126	139.6(11)	133(5)	135	145(8)	8.5	8.6(1)
200	74.6	77.50(4)	82(10)	75.1	78.2(4)	0.52	0.50(−3)
400	41.4	41.08(−0.8)	46(11)	41.4		0.019	
800	22.8	22.88(0.3)		22.8		0.0006	

TABLE XI. Coupled-Sturmian cross sections (in units of 10^{-19} cm^2) for ionization and direct excitation versus proton energy E (in units of MeV) in p-H collisions using the single-center basis $\leq 30(s,p,d,f)$ on the target (280 states). Numbers in parentheses are percent differences (before rounding) from results with the first Born approximation (for consistency with only s,p,d,f waves for ionization).

E	Ionization	$2s$	$3s$	$4s$	$2p$	$3p$	$4p$	$3d$	$4d$
0.5	342(−0.2)	20.2(5)	4.09(7)	1.53(8)	332.(−3)	56.1(−3)	19.8(−3)	3.13(9)	1.49(9)
0.6	292(−0.5)	16.8(4)	3.39(6)	1.27(7)	292.(−2)	49.2(−2)	17.4(−2)	2.58(7)	1.22(7)
1	188(−0.9)	9.93(2)	1.99(3)	0.743(4)	202.(−1)	33.8(−1)	11.9(−1)	1.51(4)	0.717(4)
2	103(−1)	4.92(1)	0.980(1)	0.365(2)	118.(−0.5)	19.7(−0.5)	6.94(−0.5)	0.748(1)	0.354(1)
4	55.7(−1)	2.45(0.5)	0.487(0.6)	0.181(0.6)	67.8(−0.2)	11.2(−0.2)	3.95(−0.2)	0.373(0.5)	0.177(0.6)
8	30.0(−1)	1.22(0.2)	0.243(0.2)	0.090(0.3)	38.1(−0.1)	6.30(−0.1)	2.21(−0.1)	0.186(0.2)	0.088(0.2)
9.6	25.5(−1)	1.02(0.2)	0.203(0.2)	0.075(0.2)	32.7(−0.1)	5.40(−0.07)	1.90(−0.06)	0.155(0.1)	0.074(0.1)
16	16.1(−1)	0.611(0.1)	0.121(0.1)	0.045(0.1)	21.2(−0.05)	3.49(−0.05)	1.22(−0.04)	0.093(0.1)	0.044(0.1)

shown) rather than a 280-state basis. The Born ionization and the single-center Sturmian ionization curves cross between 400 and 500 keV, with the Sturmian cross section lying 1% *above* the Born cross section at 300 keV and 4% above at 200 keV (not shown). Within the first Born approximation for ionization including partial waves through h, the contribution from the p wave increases monotonically with energy from 65% at 0.5 MeV to 76% at 16 MeV, while the contribution from each of the other partial waves decreases, the g contribution, from 2.5% to 1.6%, and the h contribution, from 1.3% to 0.9%.

Values at 0.6 and 9.6 MeV have been included in order to compare with those reported by the author [10] for α-H collisions at the same energies in units of MeV/u. The first Born cross sections for direct excitation and ionization scale exactly with the square of the projectile charge, and thus for α-H collisions are four times larger. For 0.6 MeV p-H collisions, the 280-state cross sections are seen in the present table to agree with Born cross sections to 4–7 % for s states, 2% for p states, 7% for d states, and 0.5% for ionization, versus 2–6 %, 9%, 28%, and 0.9%, respectively, for 0.6 MeV/u α-H collisions. For 9.6 MeV p-H collisions, the 280-state and the Born cross sections for s,p,d excitation and for ionization agree to 0.2%, $\leq$0.1%, 0.1%, and 1%, respectively, versus 0.1–0.3 %, 0.3–0.4 %, 0.7%, and 1%, respectively, for 9.6 MeV/u α-H collisions. These differences for different projectile charges reflect the fact that the scaling with the square of projectile charge is only approximate for the coupled-state calculations at any energy—indeed, with the 280-state basis, at 0.6 MeV/u, the scaled individual-state s,p,d excitation and ionization cross sections for p-H and α-H collisions agree to (only) 1–2 %, 7%, 16%, and 0.3%, respectively; these differences between the scaled p-H and α-H cross sections decrease to $<$0.1%, 0.2–0.3 %, 0.5–0.6 %, and 0.1% by 9.6 MeV/u.

IV. CONCLUSION

The original small-basis Sturmian cross sections of Shakeshaft [7,8] have been checked to be numerically correct but nonconverged by as much as 30–40 % for transfer or excitation to some states up to $n=3$. In contrast, the present calculations use three large Sturmian bases over a wide range of energies, whose convergence has been studied. At lower of energies 1–100 keV, the two symmetric bases $\leq 16(s,p,d)$ and $\leq 13(s,p,d,f)$ on each center (respectively, 176 and 220 Sturmians in all) yield capture and excitation cross sections up to $3d$, as well as ionization cross sections, generally estimated to be converged to at least 5%, with noted exceptions. There is a close agreement at the low energies of 1 and 4 keV with the 394-Gaussian results of Toshima [16]. At 100 keV, the cross sections tie into those obtained with an asymmetric basis of 281 Sturmians centered almost entirely on the target—a basis appropriate at the higher energies.

Several questions regarding other theoretical and experimental results have been addressed. First, the present Sturmian results confirm that at low energies the capture and excitation cross sections for a given $n\ell$ do merge, and thus the $2p$ disparity for one coupled-state calculation [23] cannot be explained. Second, the present Sturmian results for the Balmer-alpha excitation confirm other existing large-basis results, and thus a large discrepancy persists with the experimental cross section [26]. Third, at peak and somewhat higher energies, the present Sturmian ionization cross section agrees within 2% with the 394-Gaussian cross section [16], with both cross sections being at least 25% above the experimental cross section [29]. Fourth, the $2p$ alignment has been calculated at the sensitive energies where it passes through zero, reducing but still leaving a significant discrepancy with the experimental results [54]. Fifth, the present and other theoretical $2p$ capture cross sections show some disagreement in shape at lower energies and in magnitude at higher energies with the experimental results [46,47]. Sixth, the present and some other theoretical $2s$ excitation cross sections lie about 20% above the experimental values at higher energies [51]. Considering the fundamental nature of p-H collisions, it would be very useful for additional experiments, as well as calculations, to address these questions.

ACKNOWLEDGMENTS

I thank Robert Forrey for insight on the convergence of large Sturmian bases and Serguei Ovchinnikov for emphasizing the challenge of obtaining accurate theoretical peak ionization cross sections.

[1] D. R. Bates, Proc. R. Soc. London, Ser. A **247**, 294 (1958).
[2] R. McCarroll, Proc. R. Soc. London, Ser. A **264**, 547 (1961).
[3] I. M. Cheshire, D. F. Gallaher, and A. J. Taylor, J. Phys. B **3**, 813 (1970).
[4] T. G. Winter and C. C. Lin, Phys. Rev. A **10**, 2141 (1974).
[5] D. F. Gallaher and L. Wilets, Phys. Rev. **169**, 139 (1968).
[6] R. Shakeshaft, J. Phys. B **8**, 1114 (1975).
[7] R. Shakeshaft, Phys. Rev. A **14**, 1626 (1976).
[8] R. Shakeshaft, Phys. Rev. A **18**, 1930 (1978).
[9] T. G. Winter, Phys. Rev. A **25**, 697 (1982).
[10] T. G. Winter, Phys. Rev. A **76**, 062702 (2007).
[11] A. F. Ferguson, Proc. R. Soc. London, Ser. A **264**, 540 (1961).
[12] D. R. Bates and D. A. Williams, Proc. Phys. Soc. Lond. **83**, 425 (1964).
[13] S. K. Knudson and W. R. Thorson, Can. J. Phys. **48**, 313 (1970).
[14] R. McCarroll and R. D. Piacentini, J. Phys. B **3**, 1336 (1970).
[15] J. Kuang and C. D. Lin, J. Phys. B **29**, 1207 (1996).
[16] N. Toshima, Phys. Rev. A **59**, 1981 (1999).
[17] A. L. Ford, J. F. Reading, and K. A. Hall, J. Phys. B **26**, 4537 (1993).
[18] M. Kimura and W. R. Thorson, Phys. Rev. A **24**, 1780 (1981).
[19] S. Zou, L. Pichl, M. Kimura, and T. Kato, Phys. Rev. A **66**, 042707 (2002).
[20] D. G. M. Anderson, M. J. Antal, and M. B. McElroy, J. Phys. B **7**, L118 (1974); **14**, 1707(E) (1981).
[21] T. G. Winter and C. D. Lin, Phys. Rev. A **29**, 567 (1984).
[22] T. G. Winter and C. D. Lin, Phys. Rev. A **29**, 3071 (1984); **30**, 3323(E) (1984).
[23] B. M. McLaughlin, T. G. Winter, and J. F. McCann, J. Phys. B **30**, 1043 (1997).
[24] C. D. Lin (private communication).
[25] T. G. Winter, Adv. At., Mol., Opt. Phys. **52**, 391 (2005).
[26] A. Donnelly, J. Geddes, and H. B. Gilbody, J. Phys. B **24**, 165 (1991).
[27] H. A. Slim, J. Phys. B **26**, L743 (1993).
[28] S. Ovchinnikov (private communication).
[29] M. B. Shah, D. S. Elliott, and H. B. Gilbody, J. Phys. B **20**, 2481 (1987).
[30] F. Melchert, S. Krüdener, R. Schulze, S. Petri, S. Pfaff, and E. Salzborn, J. Phys. B **28**, L355 (1995).
[31] C. Y. Chen, C. L. Cocke, J. P. Giese, F. Melchert, I. Reiser, M. Stöckli, E. Sidky, and C. D. Lin, J. Phys. B **34**, 469 (2001).
[32] This equation (given in a somewhat more general form) has also been derived in a classical Liouville formalism [C. O. Reinhold and C. A. Falcón, J. Phys. B **21**, 1829 (1988)].
[33] A. Kołakowska, M. S. Pindzola, F. Robicheaux, D. R. Schultz, and J. C. Wells, Phys. Rev. A **58**, 2872 (1998).
[34] D. R. Bates and G. Griffing, Proc. Phys. Soc., London, Sect. A **66**, 961 (1953); D. R. Bates, in *Atomic and Molecular Processes*, edited by D. R. Bates (Academic, New York, 1962), pp. 550–556.
[35] The first parameters are $z_{\min}=-200a_o$, $z_{\max}=2000a_o$, $R_{\max}=50a_o$, $N_\lambda=32$, $N_\mu=40$, and $\rho=0(0.15)3.6(0.3)20.4a_o$; the second (more stringent) parameters are $e_1,e_2=10^{-8,-6}$, $z_{\min}=-2000a_o$, $z_{\max}=3000a_o$, $R_{\max}=100a_o$, $N_\lambda\geq 40$, $N_\mu\geq 80$, and $\rho=0(0.1)3.6(0.2)25.6a_o$.
[36] The 92-Sturmian parameters are $z_{\min}=-200a_o$, $z_{\max}=2000a_o$, $R_{\max}=120a_o$, $N_\lambda\geq 40$, $N_\mu\geq 80$, and $\rho=0(0.3)3.6(0.6)20.4a_o$. The error in the summed cross section is $|\Sigma Q-\pi\rho_{\max}^2|\leq 0.000\,04\times10^{-17}$ cm^2 for $E\geq 70$ keV and $\leq 0.0009\times10^{-17}$ cm^2 at lower energies.
[37] The 176- (and 140-) Sturmian parameters differing from those of the reference (68-Sturmian) basis (in Sec. II A 1) are $-z_{\min}=R_{\max}=120a_o$, $N_\lambda\geq 32$, and $N_\mu\geq 40$, while $z_{\max}$ and the ρ's are the same. The error in the summed cross section is again small: $|\Sigma Q-\pi\rho_{\max}^2|\leq 0.001\times10^{-17}$ cm^2 (except 0.003×10^{-17} cm^2 at 75–100 keV) and may independently confirm the numerical accuracy of the cross sections to the tabulated number of digits except for $3d$ transfer at 75–100 keV.
[38] The 281-Sturmian parameters are $-z_{\min}=z_{\max}=1000a_o$, $R_{\max}=60a_o$, $N_\lambda\geq 40$, $N_\mu=24$, and $\rho=0(0.3)3.6(0.6)6(1.2)\rho_{\max}$, with $\rho_{\max}$ increasing from $20.4a_o$ at 100 keV to $49.2a_o$ at 1000 keV. The error in the summed cross section is small: $|\Sigma Q-\pi\rho_{\max}^2|\leq 0.0001\times10^{-18}$ cm^2 for $E\geq 200$ keV and 0.0008×10^{-18} cm^2 at 100 keV.
[39] The use of smaller values of $n_{\max}$ than in the production runs (with $n_{\max}=30$) does not much affect cross sections except for $4s$, which is not converged here; however, the effect of g states on $4s$ appears negligible, consistent with its negligible effect on the more accurately represented (lower) s states. The 141-state cross sections were obtained using the same parameters as with the 281-Sturmian production basis [38] (except for a coarser ρ mesh up to $1.2a_o$ to reduce the CPU time, which, however, has only a slight effect on the accuracy). The 185-state cross sections were obtained using the same z range and ρ's as with the 281-Sturmian basis, except that now $\rho_{\max}$ is increased further at very high energies [58].
[40] H. J. Lüdde and R. M. Dreizler, J. Phys. B **15**, 2703 (1982).
[41] G. W. McClure, Phys. Rev. **148**, 47 (1966).
[42] W. Fritsch and C. D. Lin, Phys. Rev. A **26**, 762 (1982).
[43] W. Fritsch and C. D. Lin, Phys. Rev. A **27**, 3361 (1983).
[44] E. Y. Sidky and C. D. Lin, Phys. Rev. A **65**, 012711 (2001).
[45] J. E. Bayfield, Phys. Rev. **185**, 105 (1969).
[46] T. Kondow, R. J. Girnius, Y. P. Chong, and W. L. Fite, Phys. Rev. A **10**, 1167 (1974).
[47] T. J. Morgan, J. Geddes, and H. B. Gilbody, J. Phys. B **6**, 2118 (1973).
[48] Y. P. Chong and W. L. Fite, Phys. Rev. A **16**, 933 (1977).
[49] J. Hill, J. Geddes, and H. B. Gilbody, J. Phys. B **12**, L341 (1979).
[50] T. J. Morgan, J. Stone, and R. Mayo, Phys. Rev. A **22**, 1460 (1980).
[51] D. P. Higgins, J. Geddes, and H. B. Gilbody, J. Phys. B **29**, 1219 (1996).
[52] D. Detleffsen, M. Anton, A. Werner, and K.-H. Shartner, J. Phys. B **27**, 4195 (1994).
[53] M. P. Hughes, J. Geddes, R. W. McCullough, and H. B. Gilbody, Nucl. Instrum. Methods Phys. Res. B **79**, 50 (1993).
[54] R. Hippler, H. Madeheim, W. Harbich, H. Kleinpoppen, and H. O. Lutz, Phys. Rev. A **38**, 1662 (1988).
[55] T. G. Winter and C. D. Lin (unpublished).
[56] The effect of g states on the ionization cross section is difficult to establish directly in the present Sturmian calculations: for example, whereas the change in the 1 MeV ionization cross section on increasing a purely one-center basis from $\leq 12(s,p,d,f)$ to $\leq 12(s,p,d,f,g)$ is only 0.04%, the change from $\leq 15(s,p,d,f)$ to $\leq 15(s,p,d,f,g)$ is 0.13%. It would take an impractically large Sturmian basis in the present form to establish the converged ionization limit including g states, owing to the long-range behavior of g waves.

[57] To test the convergence with respect to n_{max}, cross sections were also calculated at 1, 2, 4, 8, and 16 MeV with the single-center bases $\leq 35(s,p,d,f)$ (330 states) and $\leq 40(s,p,d,f)$ (380 states); except for ionization, the changes are in at most the fourth digit and are smaller on going from the 330- to the 380-state basis than from the 280- to the 330-state basis.

[58] These Born results were obtained here in the impact-parameter version using the same impact parameters as in the coupled-Sturmian approach, with ρ_{max} increasing with energy to $202.8a_o$ by 16 MeV due to the increasingly long-range behavior of p excitation and p-wave ionization as well as, to some extent, d-wave ionization. The 280-Sturmian cross sections were obtained using the same ρ's (now extended at high energy) and z range as with the 281-Sturmian basis [38] (with a slightly coarser ρ mesh at 0.6 and 9.6 MeV). For excitation, halving the ρ mesh at 1, 4, and 16 MeV changes the Born results (and presumably the coupled-state results) in at most the fourth digit, except for $4d$ at 1 MeV and $3d$ at 16 MeV, for which, however, the changes are only 0.2%. As a further test, the z range in the 280-Sturmian calculation was increased by a factor of 5 to $-z_{min}=z_{max}=5000a_o$ at each energy from 1 to 16 MeV, with the maximum change in any cross section being 1 unit in the last reported digit.