

# Ionization and excitation in collisions between antiprotons and H(1s) atoms studied with Sturmian bases

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Coupled two-center as well as one-center Sturmian cross sections have been determined for ionization and excitation in  $\bar{p}$ -H(1s) collisions at  $\bar{p}$  energies from 1 to 16 000 keV, following the author's recent work for  $p$ -H(1s) collisions [Phys. Rev. A **80**, 032701 (2009)]. Basis convergence is studied in detail. Results for ionization and excitation are compared to other coupled-state results and to numerical results, as well as limited experimental results for ionization only. Except for the large, two-center coupled-Gaussian-pseudostate calculation of Toshima for ionization only [Phys. Rev. A **64**, 024701 (2001)], previous calculations employed one-center bases, including a one-center Sturmian calculation by Igarashi *et al.* [Phys. Rev. A **61**, 062712 (2000)]. A strong contrast with  $p$ -H collisions is confirmed at intermediate energies, while at high energies the extent of agreement is revealed between coupled-state results for the two collisional systems, as well as with first Born results.

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## I. INTRODUCTION

Electronic transitions in  $p$ -H and  $\bar{p}$ -H collisions are fundamental atomic collision processes. These and other one-electron collision processes can be treated at intermediate (keV) energies with considerable accuracy. (A proton or antiproton moving at the Bohr velocity  $c/137$  has a kinetic energy of 25 keV.) The  $p$ -H process has recently been considered by the author [1], and earlier work on this and other one-electron ion-atom collisions has been reviewed [2]. An account of work on  $\bar{p}$ -H collisions may be found in the recent paper by McGovern *et al.* [3].

The fundamental difference between the two collisions is the absence of the capture channel in  $\bar{p}$ -H collisions; the electron can only be ionized or excited to higher bound states. This has led researchers to use one-center bases in solving the time-dependent Schrödinger equation with a coupled-state approach—the largest by McGovern *et al.* [3], Hall *et al.* [4], Schiwietz *et al.* [5], and Igarashi *et al.* [6], the last using a Sturmian basis.

A single researcher, Toshima, used a two-center basis (specifically, a large two-center Gaussian basis) [7]. He noticed a substantial difference between one- and two-center ionization cross sections at low energies and argued that only projectile-centered functions could account for the spreading out of the electron cloud at large distances from the projectile. And at intermediate energies he noted a dip in the electron density in the vicinity of the projectile, a dip absent in the one-center treatments. The same delocalization of the electron cloud in the vicinity of the antiproton was noted by Wells *et al.* [8] in numerically solving the time-dependent Schrödinger equation. Another numerical calculation has been reported by Sakimoto [9].

Accordingly, despite the absence of capture channels, two-center bases have been used here: specifically, the same symmetric two-center Sturmian bases have been used as in the  $p$ -H paper [1]; the same basis functions have been placed on the antiproton as on the proton. This choice is intended to provide in a simple way for variational freedom beyond that of a one-center basis, and allow a description of the mechanisms just noted. In a one-center basis, without using a large number

of high-angular-momentum basis functions centered on the target proton, it would be expected to be difficult to describe accurately either a buildup or a deficiency of the electron cloud centered on the antiproton. In a two-center basis, the precise form of the basis functions centered on the antiproton is probably unimportant; it is only desirable that the basis can be changed in a simple and systematic way. The two-center basis is overly complete in the large-basis limit, but for finite bases some improvement might be found with the addition of a set of basis functions on the second center.

The outline of the paper is as follows. In Sec. II the method will be presented, numerical accuracy assessed, basis convergence studied, and results summarized. In Sec. III the results will be compared to other theoretical results and limited experimental results. Conclusions will be drawn in Sec. IV.

## II. METHOD

As in Ref. [1] and following Shakeshaft [10], the Sturmian basis functions on each center are simply polynomials in the radial electronic variable  $r$  multiplied by a *fixed* exponential  $e^{-Zr/[(\ell+1)a_0]}$  (and a spherical harmonic). The polynomials and hence the Sturmians form a complete set. For H (and other hydrogenic atoms), each of the lowest electronic states  $1s, 2p, 3d, \dots$  of different angular momenta  $\ell$  can be represented exactly by a single Sturmian. For  $p$ -H collisions [1], we have  $Z = 1$  for both centers, halving the number of distinct matrix elements at each time step. The same choice has been made for  $\bar{p}$ -H collisions, leading to a similar savings. Separated H-atom ( $pe$ ) states with positive Hamiltonian eigenvalues are ionization states. *All* Hamiltonian eigenvalues of the separated  $\bar{p}e$  system are positive, and so also correspond to ionization states.

In their one-center  $\bar{p}$ -H calculations with large Sturmian bases, Igarashi *et al.* [6] set the exponential constant  $Z/(\ell+1)$  instead to be the fixed value 0.6, independent of  $\ell$ . Their Sturmians are thus longer range for  $s$  states and shorter range for states of higher  $\ell$  than the present choice. Shakeshaft, as a follow-up to his original two-center Sturmian calculations noted above, had also used “scaled Sturmians” [11] for  $p$ -H

collisions, Sturmians with a fixed value  $Z/(\ell + 1) < 1$  in the exponent.

## A. Numerical tests

### 1. Integration parameters

As in Ref. [1] and the author's earlier work, the two-center scattering program has the following parameters: (1) the truncation-error limits  $e_1, e_2$  for the transition coefficients and (2) the limits  $z_{\min}, z_{\max}$  in integrating the coupled equations for the coefficients over  $z = vt$  (the absolute square of each coefficient at  $z_{\max}$  being the corresponding transition probability) and (3) the limiting internuclear distance  $R_{\max}$  and (4) the number of integration points  $N_\lambda, N_\mu$  in evaluating the charge-exchange matrix elements in the spheroidal coordinates  $\lambda, \mu$ ; and (5) the impact parameters  $\rho$  in integrating probability times  $\rho$  over  $\rho$  to obtain the cross section. [In the one-center calculations, parameters (3) and (4) are irrelevant.] The following parameters have been chosen here:  $e_1, e_2 = 10^{-7}, -5$ ,  $z_{\min} \approx -100a_0, z_{\max} = 1000a_0$  [12],  $R_{\max} = 120a_0$  (except  $150a_0$  at energies up to 5 keV),  $N_\lambda = 32, N_\mu = 40$  (but  $N_\lambda = 52, N_\mu = 96$  at energies of at least 15 keV),  $\rho = 0(0.3)3.6(0.6)6(0.6 \text{ or } 1.2)\rho_{\max}$  (in units of  $a_0$ ), where  $\rho_{\max} = 10.8a_0$  at the lower energies, increasing to  $34.8a_0$  at 20 keV, with still higher values of  $\rho_{\max}$  above 400 keV [13]. This choice of parameters has been tested by comparing cross sections to values obtained with other choices, indicating that almost all cross sections reported here are *numerically* accurate to at least 0.5%, and certainly to 1%, with the exception of a few percent sensitivity of the small  $3s$  two-center cross section to  $N_\lambda$  at the higher energies, where it is only reported to one digit. The chosen parameters are similar to, or more stringent than, those used in Ref. [1].

### 2. Summed cross section

As in Ref. [1], a simple independent test of sensitivity to the parameters has also been introduced. Since probability should be conserved in integrating the coupled equations, the summed cross section  $\Sigma Q$  (including the elastic channel) should be identical to  $\pi\rho_{\max}^2$ , but it is not, due to small numerical errors. In the present case, the *relative* error in  $\Sigma Q$  usually [14] does not exceed 0.0007%. The *absolute* error in  $\Sigma Q$  is consistent with the absolute sensitivity in the individual cross sections, which are tabulated to an appropriate precision. The error in  $\Sigma Q$  reflects the choice of  $e_1, e_2, R_{\max}, N_\lambda, N_\mu$ , but only indirectly the choice of  $\rho$  or  $z$  range.

### 3. Highest $s$ state

As in Refs. [1,11], the present calculations neglect the highest  $s$  state on each center after diagonalizing the atomic Hamiltonians. The highest  $s$  state has a very high positive energy and negligible cross section, and, were it included, coupling to it would slow the computation by about a factor of two.

## B. Convergence tests

### 1. Two-center, symmetric $s, p, d$ basis

A test of convergence of the present symmetric two-center Sturmian cross sections within the  $s, p, d$  manifold is given in

Table I, as in Ref. [1] for  $p$ -H collisions. Shown are absolute differences of cross sections using the basis  $\leq 16(s, p, d)$  on each center (176 states in all) (except where noted) from values obtained with the basis  $\leq 13(s, p, d)$  on each center (140 states in all). [A basis  $\leq n(s, p, d)$  includes Sturmians from  $1s$  to  $ns$ ,  $2p$  to  $np$ , and  $3d$  to  $nd$ .] Where exceeding one unit in the last digit, they are  $\leq 4\%$ , except for  $3s$  (31, 19, 12%) and  $3p$  (14, 7, 6%) at 1, 2, 3 keV, respectively, and  $2s, 3p$  (6–7 %) and  $3d$  (10–12 %) for some energies in the range 50–100 keV. The numerical error estimate in the last column of Table I is the absolute difference of the cross section summed over all channels (including the elastic channel) from  $\pi\rho_{\max}^2$ ; it is seen to be negligible compared to the cross-section digits reported here.

### 2. Two-center, symmetric $s, p, d, f$ basis

As in Ref. [1], convergence with respect to increasing the maximum angular momentum quantum number  $\ell_{\max}$  has also been tested: Shown in Table II are cross sections with the basis  $\leq 13(s, p, d, f)$  on each center (220 states in all), together with differences from values obtained with the basis  $\leq 13(s, p, d)$  on each center (140 states in all, the same reference basis as in the preceding section). Where exceeding one unit in the last digit, they are  $\leq 4\%$ , except for  $3p, 3d$  at 2 keV (11–12 %) and  $3d$  for some energies in the range 15–100 keV (10–17 %) [15]. The numerical error estimate in the last column is negligible compared to the cross-section digits reported, except at 2 keV.

### 3. One-center $s, p, d, f$ basis

It has been noted [1] for  $p$ -H collisions that the symmetric two-center Sturmian bases cannot be enlarged much further than the above 176-state  $(s, p, d)$  and 220-state  $(s, p, d, f)$  bases, for at least two reasons: First, at lower energies the computing time becomes large due to the small  $z$ -step size required owing to the rapidly varying energy phases; further, the matrix elements, like the energy phases, are proportional to  $1/v$ . Computing, as for  $p$ -H collisions [1], is done on a 3.3 GHz IBM ThinkPad; computing times are comparable for the two collisional systems, except at low energies, where the present ( $\bar{p}$ -H) calculations are slower (taking up to about 100 h at the lowest energy), perhaps owing to the very strong, diffuse ionization channel. The second reason the two-center Sturmian bases cannot be enlarged much further is that at higher energies a high-order quadrature (and hence increased computing time) is required to evaluate the charge-exchange matrix elements with their rapidly varying velocity-dependent translational factors.

However, at higher energies for  $p$ -H collisions a large basis is achievable by simply neglecting the then insignificant capture channels. As noted in Sec. I, this has been proposed by several researchers for  $\bar{p}$ -H collisions at all energies, since there is no capture. Accordingly, in Table III are presented cross sections using the one-center Sturmian basis  $\leq 30(s, p, d, f)$  centered on the target proton (280 states), as in [1] for  $p$ -H collisions, but now at lower energies as well. As in that paper,  $n = 4$  excitation cross sections are also reported. Igarashi *et al.* [6] have also reported one-center Sturmian calculations, calculations with more  $\ell$  but fewer  $n$ ; these results

TABLE I. Coupled-Sturmian cross sections (in units of  $10^{-17}$  cm<sup>2</sup>) for ionization and excitation in  $\bar{p}$ -H collisions using the basis  $\leq 16(s, p, d)$  on each center (176 states in all), except using the basis  $\leq 15(s, p, d)$  on each center (164 states in all) at 1–2 keV to reduce the computing time. Numbers in parentheses are the differences in the last digit(s) from values obtained with the basis  $\leq 13(s, p, d)$  on each center (140 states in all). The error estimate is an absolute numerical error estimate (in the same units as the cross sections).

| $E$ (keV) | Ionization | 2s       | 3s       | 2p       | 3p       | 3d       | all <sup>a</sup> | Error   |
|-----------|------------|----------|----------|----------|----------|----------|------------------|---------|
| 1         | 11.42(16)  | 1.46(−1) | 0.22(5)  | 1.70(0)  | 0.52(−9) | 0.26(1)  | 5.82(−16)        | 0.001   |
| 2         | 12.15(−4)  | 1.31(1)  | 0.19(3)  | 2.52(0)  | 0.60(−4) | 0.37(1)  | 6.72(3)          | 0.002   |
| 3         | 12.73(20)  | 1.23(−1) | 0.19(2)  | 3.06(1)  | 0.62(−4) | 0.43(0)  | 7.20(−20)        | 0.002   |
| 5         | 13.33(6)   | 1.15(0)  | 0.18(1)  | 3.84(−1) | 0.68(−3) | 0.50(1)  | 8.03(−7)         | 0.00007 |
| 10        | 14.01(7)   | 0.99(0)  | 0.16(0)  | 5.14(−1) | 0.81(−1) | 0.56(1)  | 9.32(−8)         | 0.003   |
| 15        | 14.11(9)   | 0.88(0)  | 0.14(−1) | 5.99(0)  | 0.91(0)  | 0.57(−1) | 10.17(−9)        | 0.003   |
| 25        | 13.80(0)   | 0.74(0)  | 0.11(−1) | 7.01(2)  | 1.07(1)  | 0.53(0)  | 11.13(−2)        | 0.001   |
| 50        | 12.39(10)  | 0.59(2)  | 0.09(−1) | 7.83(−4) | 1.22(−9) | 0.38(0)  | 11.68(−13)       | 0.007   |
| 75        | 10.86(−20) | 0.50(−4) | 0.08(0)  | 7.75(6)  | 1.32(1)  | 0.26(3)  | 11.38(9)         | 0.002   |
| 100       | 9.79(−10)  | 0.47(−1) | 0.08(−1) | 7.33(6)  | 1.15(−8) | 0.22(2)  | 10.55(−4)        | 0.0006  |
| 200       | 6.56(19)   | 0.32(−1) | 0.06(−1) | 5.69(−5) | 0.99(4)  | 0.09(−1) | 8.13(−2)         | 0.003   |

<sup>a</sup>All available bound excited states.

TABLE II. Coupled-Sturmian cross sections (in units of  $10^{-17}$  cm<sup>2</sup>) for ionization and excitation in  $\bar{p}$ -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 obtained with the basis  $\leq 13(s, p, d)$  on each center (140 states in all). The error estimate is an absolute numerical error estimate (in the same units as the cross sections).

| $E$ (keV) | Ionization | 2s       | 3s       | 2p        | 3p       | 3d       | all <sup>a</sup> | Error  |
|-----------|------------|----------|----------|-----------|----------|----------|------------------|--------|
| 2         | 12.11(−8)  | 1.31(1)  | 0.16(0)  | 2.51(−1)  | 0.57(−7) | 0.40(4)  | 6.79(10)         | 0.03   |
| 3         | 12.48(−6)  | 1.24(0)  | 0.17(0)  | 3.06(1)   | 0.63(−3) | 0.44(1)  | 7.46(6)          | 0.003  |
| 5         | 13.20(−7)  | 1.15(0)  | 0.17(0)  | 3.85(0)   | 0.70(−1) | 0.49(0)  | 8.17(7)          | 0.0004 |
| 10        | 13.82(−12) | 0.99(0)  | 0.16(0)  | 5.15(0)   | 0.83(1)  | 0.53(−2) | 9.49(9)          | 0.0009 |
| 15        | 14.00(2)   | 0.88(0)  | 0.14(−1) | 5.99(0)   | 0.94(3)  | 0.51(−7) | 10.27(1)         | 0.004  |
| 25        | 13.83(3)   | 0.74(0)  | 0.12(0)  | 6.99(0)   | 1.09(3)  | 0.48(−5) | 11.11(−4)        | 0.001  |
| 50        | 12.40(11)  | 0.59(2)  | 0.09(−1) | 7.76(−11) | 1.33(2)  | 0.32(−6) | 11.69(−12)       | 0.003  |
| 75        | 11.12(6)   | 0.53(−1) | 0.08(0)  | 7.64(−5)  | 1.26(−5) | 0.24(1)  | 11.20(−9)        | 0.003  |
| 100       | 9.95(6)    | 0.48(0)  | 0.09(0)  | 7.19(−8)  | 1.22(−1) | 0.18(−2) | 10.49(−10)       | 0.007  |
| 200       | 6.52(14)   | 0.33(0)  | 0.06(0)  | 5.69(−5)  | 0.95(0)  | 0.10(0)  | 8.10(−5)         | 0.008  |

<sup>a</sup>All available bound excited states.

TABLE III. Coupled-Sturmian cross sections (in units of  $10^{-18}$  cm<sup>2</sup>) for ionization and excitation in  $\bar{p}$ -H collisions using the one-center basis  $\leq 30(s, p, d, f)$  on the target proton (280 states). Numbers in parentheses are differences in the last digit(s) from values obtained with the one-center basis  $\leq 25(s, p, d, f)$  (230 states).

| $E$ (keV) | Ioniz.   | 2s       | 3s        | 4s       | 2p       | 3p       | 4p       | 3d        | 4d        | 4f         |
|-----------|----------|----------|-----------|----------|----------|----------|----------|-----------|-----------|------------|
| 5         | 135.(0)  | 11.18(2) | 2.08(18)  | 0.74(−3) | 38.8(−1) | 6.4(−3)  | 1.96(12) | 4.84(13)  | 2.39(−24) | 0.54(5)    |
| 10        | 142.(1)  | 9.79(9)  | 1.61(13)  | 0.61(−4) | 51.0(−3) | 8.7(−2)  | 2.71(13) | 4.65(1)   | 2.25(−13) | 0.49(−6)   |
| 20        | 144.(0)  | 8.71(−2) | 1.22(5)   | 0.39(1)  | 63.5(2)  | 10.4(−2) | 3.56(−1) | 4.65(3)   | 2.04(−1)  | 0.43(−3)   |
| 30        | 140.(−1) | 7.66(5)  | 1.15(−2)  | 0.36(−2) | 71.2(−1) | 11.1(1)  | 3.76(6)  | 4.72(−6)  | 2.09(−2)  | 0.34(0)    |
| 40        | 135.(−1) | 6.70(−5) | 1.07(1)   | 0.35(0)  | 76.2(2)  | 11.7(−1) | 3.91(0)  | 4.42(9)   | 2.03(2)   | 0.23(2)    |
| 50        | 129.(−1) | 6.04(1)  | 0.968(8)  | 0.33(1)  | 78.6(1)  | 12.2(−1) | 4.10(−2) | 3.88(2)   | 1.84(1)   | 0.153(1)   |
| 60        | 123.(0)  | 5.55(4)  | 0.894(0)  | 0.30(0)  | 79.3(−1) | 12.5(0)  | 4.24(−1) | 3.39(−3)  | 1.63(−1)  | 0.108(−5)  |
| 80        | 110.(−1) | 4.88(0)  | 0.806(0)  | 0.27(−1) | 77.9(−2) | 12.6(0)  | 4.32(0)  | 2.62(−2)  | 1.27(−1)  | 0.0624(−6) |
| 100       | 99.7(−3) | 4.46(−3) | 0.753(−3) | 0.26(0)  | 74.7(−1) | 12.2(−1) | 4.24(−1) | 2.08(0)   | 1.01(0)   | 0.0399(7)  |
| 200       | 66.2(2)  | 3.23(−1) | 0.590(−3) | 0.21(0)  | 57.3(0)  | 9.62(−1) | 3.38(−1) | 0.923(−1) | 0.447(−1) | 0.0102(−1) |
| 300       | 49.5(3)  | 2.50(0)  | 0.472(−1) | 0.17(0)  | 45.8(0)  | 7.71(−1) | 2.72(0)  | 0.573(0)  | 0.276(0)  | 0.0053(0)  |
| 500       | 33.2(2)  | 1.68(−1) | 0.326(−1) | 0.12(0)  | 33.0(0)  | 5.55(−1) | 1.96(0)  | 0.323(0)  | 0.155(0)  | 0.0026(0)  |
| 1000      | 18.6(1)  | 0.92(0)  | 0.180(0)  | 0.067(0) | 20.1(0)  | 3.37(0)  | 1.19(0)  | 0.154(0)  | 0.0731(1) | 0.0011(0)  |

will be compared in Sec. III A. As a partial internal test of basis convergence in the present calculations, cross sections have been compared in Table III to those with the somewhat smaller one-center basis  $\leq 25(s,p,d,f)$  (230 states). Where exceeding one unit in the last digit, differences are  $\leq 2\%$ , except  $\leq 11\%$  for individual  $n = 3, 4$  states at 5–10 keV;  $\leq 4\%$  for  $3s, 4s$  at 20 or 30 keV; and 6–7 % for  $4f$  at 20 or 40 keV [16]. Differences oscillate with energy. The numerical error estimate [the difference of the cross section summed over all channels from  $\pi\rho_{\text{max}}^2$  (not shown in Table III)] is  $\leq 0.0001 \times 10^{-18} \text{ cm}^2$  for  $E \leq 500$  keV with the 280-state basis, and is thus negligible. The error is even smaller than that previously noted with either two-center basis, due to the absence of charge-exchange matrix elements; for a two-center approach, their approximate numerical evaluation contributed somewhat to the violation of unitarity (nonconservation of probability).

### C. Summary of results

Absolute differences between the production two-center 176- and 220-Sturmian cross sections in Tables I and II are generally small, usually  $\leq 1$  unit in the last tabulated digit and/or  $\leq 2\%$ ; more detail on percent differences is given in the next paragraph. To provide first an overview, *absolute* differences are plotted in Fig. 1. They are seen to oscillate with energy, and do not exceed about  $2 \times 10^{-18} \text{ cm}^2$ . Overall *absolute* differences are generally no greater for the individual  $n = 3$  channels than for the  $n = 2$  channels; further, differences are of smaller amplitude for  $s$  states than for  $p, d$  states. The differences for ionization and summed excitation are seen to be strongly anticorrelated, such that their combined (total inelastic) cross section difference (not shown) is negligible, except at higher energies  $\gtrsim 100$  keV. The differences for  $2p$  and  $3p$  are also somewhat anticorrelated; the summed difference for  $2p + 3p$  would be expected to be smaller than for either  $2p$  or  $3p$  separately, and the *percent* difference for the weaker channel  $3p$  would be expected to be greater than for the stronger one ( $2p$ ). The same to some extent is true of  $2s$  and  $3s$ . The total numerical error, by which is meant the absolute sum of the errors given for the two bases in Tables I and II, is, for the most part, small on the scale of Fig. 1, and therefore omitted; with the exception of some slight numerical-error contribution for  $2s, 3s$ , the figure is a true display of basis sensitivity rather than numerical sensitivity.

In relative terms, the difference of the 220-state cross sections in Table II from the 176-state cross sections in Table I is  $\leq 2\%$  for the dominant channels (ionization, excitation to the  $2p$  state, and excitation to all states) [17]. For  $3d$  it is  $\leq 18\%$ , while for  $2s, 3s, 3p$  it is usually  $\leq 6\%$  [exceptions:  $3p$  at 50 keV (9%) and  $3s$  at 2–5, 100, 200 keV (7–17 %)]. The individual-state differences have been noted to oscillate with energy. The oscillations sometimes increase in amplitude with increasing energy. Further, as has been noted, there is increasing difficulty with increasing energy of accurately calculating the two-center charge-exchange matrix elements. Thus, at energies above, say, 200 keV, a larger one-center basis is more appropriate, such as the one-center basis  $\leq 30(s,p,d,f)$  centered on the target proton (280 states), as in Ref. [1].

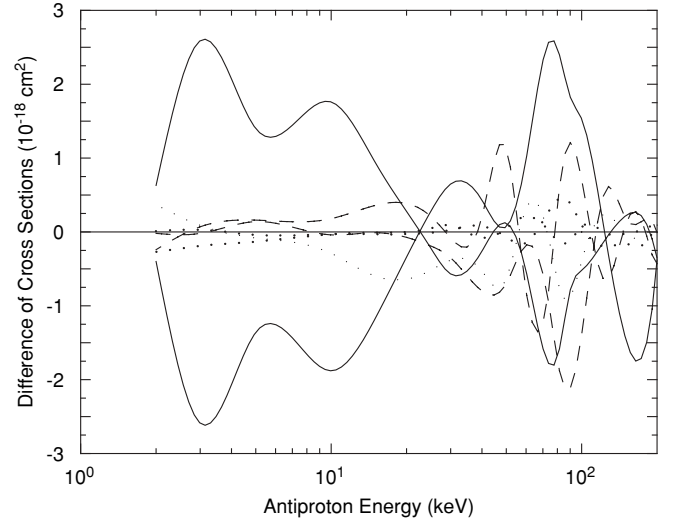


FIG. 1. Differences of two-center 220-Sturmian cross sections from two-center 176-Sturmian cross sections (164-Sturmian at 2 keV). Solid curves: excitation to all states (upper curve on the left) and ionization (lower curve); dashed curves,  $2p$  (lowest curve at 100 keV),  $3p$ ; dotted curves,  $2s, 3s$ ; thin-dotted curve,  $3d$ .

Following the work of others for  $\bar{p}$ -H collisions, this one-center basis has been used at lower energies as well; one- and two-center results may be compared at energies up to 200 keV. Differences between the present 220-state two-center and 280-state one-center cross sections are summarized as follows: The range of differences is *roughly* a factor of two greater than the range of differences between cross sections using the 220- and 176-state bases. For the three dominant processes—ionization,  $2p$  excitation, and summed excitation—*percent* differences do not exceed 4%. Except for ionization, the differences oscillate with energy, and may be (anti)correlated, as noted previously for the differences between the 220- and 176-state two-center cross sections.

The ionization, summed excitation, and individual-state excitation cross sections are plotted in Fig. 2 using the three Sturmian bases: two-center ( $s, p, d$ ) bases from 1 to 200 keV (164-state at 1–5 keV, 176-state at 3–200 keV—these differing by at most 1% at 3 and 5 keV, except for a 2.8% difference for  $3s$  at 3 keV), a two-center 220-state ( $s, p, d, f$ ) basis from 2 to 200 keV, and one-center ( $s, p, d, f$ ) bases from 5 to 16 000 keV (280-state at 5–1000 keV, 330-state at 500–16 000 keV). It is seen that results with the different bases at overlapping energies are barely distinguishable on the scale of this graph. The same would be true of a comparison of coupled-state results and first-Born results (not shown) at high energies; see Sec. III B. The  $np$  curves cross the  $ns$  curves, and dominate at higher energies; likewise the  $ns$  curves cross the  $nd$  curves, but at still higher energies, and are only slightly larger, especially for  $4s$  versus  $4d$ .

## III. COMPARISON WITH OTHER RESULTS

### A. Coupled-state and numerical results for $\bar{p}$ -H collisions

Most of the theoretical results are published in graphical form; see Figs. 3 and 4 for a rough graphical comparison with the two-center, 176-state cross sections at 1–200 keV (as



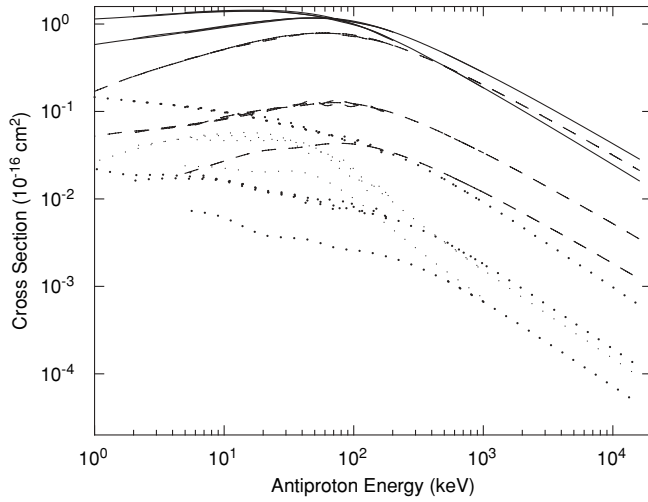


FIG. 2. Coupled-Sturmian cross sections for ionization and excitation in  $\bar{p}$ -H(1s) collisions. The upper curves from top to bottom on the far left are for ionization, excitation to all states, and excitation to the  $2p, 2s, 3p, 3d, 3s$  states. The distinct curves beginning at 5 keV are for  $4d, 4p$ , and  $4s$  from top to bottom. ( $p, s$ , and  $d$  excitations are represented by dashed, thick-dotted, and thin-dotted lines, respectively.) For clarity the  $4d$  curve is omitted above 1000 keV; by 2000 keV it is within 3% of the  $4s$  curve.

well as one-center, 280-state cross sections at energies of at least 5 keV). On the scale of the figures, the agreement is good. A more precise summary at 1–200 keV is as follows: For ionization, there are average differences of 6, 5, 2, 3, and 2 % and maximum differences of 9, 8, 6, 6, and

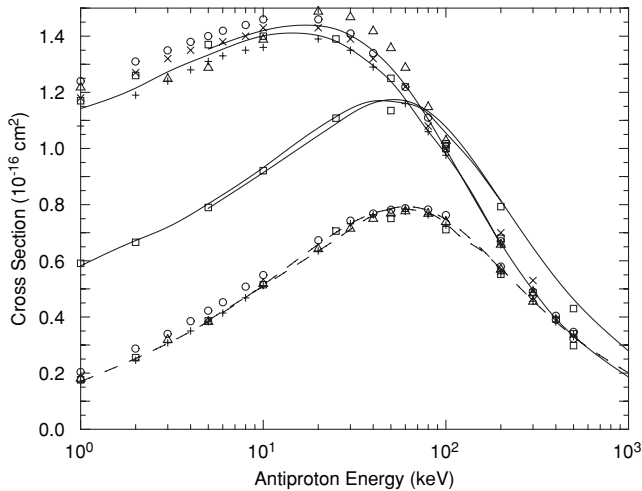


FIG. 3. Comparison with other theoretical cross sections for the three dominant processes. The present two-center, 176-Sturmian curves to 200 keV (164-Sturmian at 1, 2 keV), from top to bottom on the left are for ionization, excitation to all states, and excitation to the  $2p$  state. They are joined to the present one-center, 280-Sturmian curves at energies of at least 5 keV. The other theoretical results are as follows: Triangles, one-center coupled-pseudostate results of Hall *et al.* [4]; crosses, two-center coupled-Gaussian-pseudostate results of Toshima [7]; squares, one-center coupled-Sturmian results of Igarashi *et al.* [6]; plus signs, one-center coupled-pseudostate results of McGovern *et al.* [3]; and circles, numerical results of Sakimoto [9].

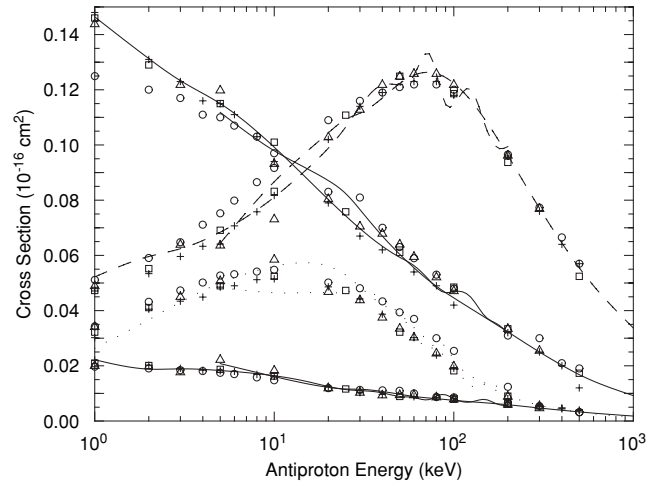


FIG. 4. Comparison with other theoretical results as in Fig. 3, but for the smaller channels  $2s, 3p, 3d, 3s$  from top to bottom on the left.

4 % from Hall *et al.* [4] (one-center-pseudostate approach), Sakimoto [9] (numerical approach), McGovern *et al.* [3] (one-center-pseudostate approach), Toshima [7] (two-center Gaussian approach), and Igarashi *et al.* [6] (one-center Sturmian approach), respectively. For excitation to the individual  $2s, 2p, 3s, 3p, 3d$  states, there are average differences of 5, 7, 4, and 5 % and maximum differences of 23, 30, 16, and 20 % from Hall *et al.*, Sakimoto, McGovern *et al.*, and Igarashi *et al.*, respectively. Maximum percent differences are usually smaller for individual  $n = 2$  states than for  $n = 3$  states.

Also the 220-Sturmian two-center cross sections may be compared at 2–200 keV with these theoretical results, as follows: For ionization, there are average differences of 5, 4, 1, 3, and 2 % and maximum differences of 9, 8, 2, 7, and 4 % from Hall *et al.*, Sakimoto, McGovern *et al.*, Toshima, and Igarashi *et al.*, respectively. For excitation to individual  $2s, 2p, 3s, 3p, 3d$  states, there are average differences of 5, 7, 5, and 3 % and maximum differences of 24, 31, 21, and 20 % from Hall *et al.*, Sakimoto, McGovern *et al.*, and Igarashi *et al.* Differences of the 220-Sturmian from the other theoretical cross sections are for the most part comparable to differences of the 176-Sturmian cross sections from them.

Finally, the 280-Sturmian one-center cross sections have been compared at 5–200 keV with these theoretical results, as follows: For ionization, there are average differences of 4, 1, 4, 2, and 2 % and maximum differences of 5, 3, 6, 5, and 3 % from Hall *et al.*, Sakimoto, McGovern *et al.*, Toshima, and Igarashi *et al.*, respectively. For excitation to individual  $2s, 2p, 3s, 3p, 3d$  states, there are average differences of 5, 6, 5, and 5 % and maximum differences of 21, 26, 14, and 21 % from Hall *et al.*, Sakimoto, McGovern *et al.*, and Igarashi *et al.*

For the dominant excitation channel ( $2p$ ) up to 200 keV, none of the three present sets of two- and one-center Sturmian cross sections differ by more than 3% from the one-center pseudostate cross sections of McGovern *et al.* at any energy. Compared instead to Igarashi *et al.*, differences do not exceed 5%, and are usually less.

The 280-Sturmian one-center cross sections, unlike the two-center Sturmian cross sections, should also be reliable at higher energies of at least 300 keV, and can thus reasonably be

compared there with the other theoretical results. Differences are generally comparable to those noted above [18].

Wells *et al.* [8] graphed their numerically determined ionization cross section up to 500 keV. Over the range 5–100 keV, the present Sturmian cross section is an average of 6–8 % (max  $\approx 10\%$ ) below theirs, regardless of which of the three Sturmian bases is used. At 500 keV the one-center 280-state cross section is 13% below theirs.

Wells *et al.* tabulated numerical cross sections for excitation to the  $2s, 2p$  states at 30, 60, and 100 keV. The present 220-Sturmian two-center cross sections differ by an average of 4% from these six values, very close to the average difference (5%) of the present cross sections from the corresponding six numerical values of Sakimoto. The maximum difference of the present values from the two sets of numerical values is 12–14 % and occurs for  $2s$  at 30 keV; the differences are, however, of opposite sign.

Finally, Hall *et al.* [4] noted good agreement between their own ionization cross sections and the large-basis one-center cross sections of Schiwietz *et al.* [5], apparently within at least 5%.

### B. Coupled-Sturmian vs Born results for $\bar{p}$ -H and $p$ -H collisions

Shown in Fig. 5 is the ratio of each cross section for antiproton impact to that for proton impact [1], using the same symmetric 176-Sturmian basis for both cases at lower energies and an asymmetric 280- or 281-Sturmian basis at higher energies. It is seen, not surprisingly, that there is a marked difference between the two processes at lower energies; at higher energies they gradually merge, as will be described in detail below. Hall *et al.* [4] have noted, using the first Born approximation as a point of reference, that at low energies the antiproton cross sections would be expected to be above the first Born cross sections, while at intermediate energies the opposite would be expected. Based on Fig. 5, the same can be said in these two energy regions of the antiproton cross sections in reference to the proton cross sections, at least for total ionization and excitation to  $s$  states. Hall *et al.* attributed the reduction in the ionization cross section at intermediate and higher energies to “antipolarization” and the enhancement of the ionization cross section at low energies to “antibinding.” Intuitively, at low energies, the slowly moving antiproton when near the target proton neutralizes it, leaving the electron to wander off.

Schultz *et al.* [19] have noted that for internuclear separations larger than the Fermi-Teller radius  $R_{FT} = 0.64a_0$  [20], the  $p\bar{p}$  dipole is sufficient to support bound molecular electronic states, but as the internuclear separation is reduced, these states correlate to states at the ionization threshold; there are no bound molecular states for smaller internuclear distances. The Fermi-Teller area  $\pi R_{FT}^2 = 3.6 \times 10^{-17} \text{cm}^2$  is thus a lower bound to the low energy  $\bar{p}$ -H ionization cross section. The ionization cross section is in fact several times larger than this, owing to transitions at larger internuclear distances from bound molecular states as well.

Shown in Table IV at the higher energies are coupled-Sturmian cross sections for ionization and excitation versus projectile energy in both  $p$ -H and  $\bar{p}$ -H collisions using the large one-center basis  $\leq 35(s, p, d, f)$  on the target (330

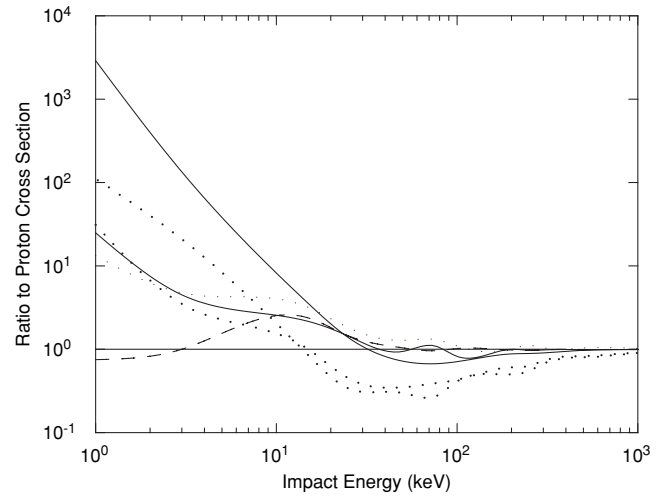


FIG. 5. Ratio of cross sections for antiproton impact to those for proton impact [1], using the same symmetric two-center 176-Sturmian basis at lower energies for both cases and asymmetric 280- or 281-Sturmian basis at higher energies. The curves from top to bottom on the left are for ionization and excitation to the  $3s, 2s, 3p, 3d, 2p$  states.

states), along with differences in each case from first Born results.

For  $2s, 3s, 4s$  excitation, the percent difference of the coupled-state cross section from the first Born cross section decreases by roughly a factor of two for each doubling of energy from 0.5 to 16 MeV (for which  $v/c \approx 0.18$ ), both for proton and antiproton impact. For antiproton impact, however, the percent differences are about twice as great as for proton impact, and of opposite sign; that is, the antiproton-impact  $s$  excitation cross sections approach the first Born cross sections from below as the energy is increased, being 0.2% below by 16 MeV, versus 0.1% above for proton projectiles. The different signs for proton and antiproton impact suggest the importance of second-Born terms, since the second-Born amplitude is proportional to  $Z^2$  rather than  $Z$ .

For  $2p, 3p, 4p$  excitation, the percent difference of the coupled-state cross section from the first Born cross section also decreases by roughly a factor of two for each doubling of energy from 0.5 to 16 MeV, both for proton and antiproton impact. However, unlike for  $s$  excitation, the differences from first Born are of about the same magnitude and the same sign for proton and antiproton impact, decreasing to 0.1% by 8 MeV. This suggests a negligible contribution from the second-Born amplitude.

For  $3d, 4d$  excitation, the percent difference of the coupled-state cross section from the first Born cross section decreases by roughly a factor of 2.5 for each doubling of energy from 0.5 to 16 MeV, both for proton and antiproton impact. For antiproton impact, however, the percent differences from Born are roughly 1.5 times as great as for proton impact, though of the same sign; that is, the antiproton-impact  $d$  excitation cross sections approach the first Born cross sections from above as the energy is increased, being 0.2% above by 8 MeV for proton impact, versus 0.3–0.4 % above for antiproton impact. Again,

TABLE IV. Coupled-Sturmian cross sections (in units of  $10^{-19} \text{ cm}^2$ ) for ionization and direct excitation versus projectile energy  $E$  (in units of MeV) in  $p$ -H collisions (upper values) and  $\bar{p}$ -H collisions (lower values) using the one-center basis  $\leq 35(s, p, d, f)$  on the target (330 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 | 344(0.2)   | 20.2(5)     | 4.09(7)     | 1.54(8)     | 332.(−3)   | 56.0(−3)   | 19.8(−3)   | 3.13(9)    | 1.48(9)    |
| 0.5 | 333 (−3)   | 16.8(−13)   | 3.26(−15)   | 1.20(−16)   | 330.(−3)   | 55.5(−4)   | 19.6(−4)   | 3.23(13)   | 1.54(14)   |
| 1   | 189 (−0.6) | 9.93(2)     | 1.99(3)     | 0.742(4)    | 202.(−1)   | 33.8(−1)   | 11.9(−1)   | 1.51(4)    | 0.717(4)   |
| 1   | 187 (−2)   | 9.15(−6)    | 1.80(−7)    | 0.666(−7)   | 201.(−1)   | 33.7(−1)   | 11.9(−2)   | 1.54(5)    | 0.731(6)   |
| 2   | 103 (−0.7) | 4.92(1)     | 0.980(2)    | 0.365(2)    | 118.(−0.5) | 19.7(−0.5) | 6.94(−0.5) | 0.748(1)   | 0.354(1)   |
| 2   | 103 (−1)   | 4.75(−2)    | 0.940(−3)   | 0.349(−3)   | 118.(−0.6) | 19.7(−0.6) | 6.93(−0.6) | 0.754(2)   | 0.357(2)   |
| 4   | 55.9(−0.7) | 2.45(0.5)   | 0.487(0.6)  | 0.181(0.7)  | 67.8(−0.2) | 11.2(−0.2) | 3.95(−0.2) | 0.373(0.5) | 0.177(0.5) |
| 4   | 55.9(−0.8) | 2.41(−1)    | 0.479(−1)   | 0.178(−1)   | 67.7(−0.2) | 11.2(−0.3) | 3.95(−0.3) | 0.374(0.8) | 0.177(0.9) |
| 8   | 30.1(−0.8) | 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) |
| 8   | 30.1(−0.8) | 1.22(−0.4)  | 0.241(−0.4) | 0.090(−0.5) | 38.1(−0.1) | 6.30(−0.1) | 2.21(−0.1) | 0.187(0.3) | 0.088(0.4) |
| 16  | 16.1(−0.7) | 0.611(0.1)  | 0.121(0.1)  | 0.045(0.1)  | 21.2(<0.1) | 3.49(<0.1) | 1.22(<0.1) | 0.093(0.1) | 0.044(0.1) |
| 16  | 16.1(−0.7) | 0.609(−0.2) | 0.121(−0.2) | 0.045(−0.2) | 21.2(<0.1) | 3.49(<0.1) | 1.22(<0.1) | 0.093(0.2) | 0.044(0.2) |

as for  $s$  but not  $p$  excitation, there is probably a significant second-Born contribution.

For  $s, d$  excitations at 0.5 MeV, where the second Born terms may be important, there are significant differences between the  $p$ -H and  $\bar{p}$ -H cross sections: about 20% for  $s$  states and 3–4 % for  $d$  states; there are still more pronounced differences at lower energies: for example, a factor of 2–3 for  $s$  states at 100 keV.

These excitation cross sections are probably largely converged with respect to increasing the maximum principal quantum number  $n_{\text{max}}$  of the Sturmian basis functions: Cross sections with  $n_{\text{max}} = 30$  (previously published for proton impact [1] and given in Table III for antiproton impact at 0.5, 1 MeV, and lower energies) rather than 35 (reported in

Table IV) are the same, save for some differences of one unit in the third digit for  $4s, 3d, 4d$ . On the other hand, the ionization cross sections are probably only converged to 1% with respect to increasing  $n_{\text{max}}$ ; the coupled-Sturmian cross sections reported here are still significantly (0.7%) below the first Born cross sections even at 16 MeV, both for proton and antiproton impact, about the same as at 2 MeV. At lower energies, the  $\bar{p}$ -H ionization cross section behaves very differently from the  $p$ -H ionization cross section, as emphasized in Fig. 5.

### C. Experimental results for ionization in $\bar{p}$ -H collisions

The only experimental cross sections for antiproton projectiles at keV energies appear to be the ionization cross sections of Knudsen *et al.* [21], which are shown in Fig. 6 along with the present two- and one-center coupled Sturmian results and previous one- and two-center coupled-state results [3,6,7]. It is seen that, within the large experimental error bars, there is general agreement between all the displayed coupled-state results and the experimental result. Not shown here are the one-center cross section of Hall *et al.* [4] and the numerical cross section of Wells *et al.* [8], which lie 7–8 % above the upper error bar of the experimental value at the lowest experimental energy, 30 keV.

## IV. CONCLUSION

Fairly large-Sturmian-basis two-center cross sections have been determined for ionization and excitation to individual states up to  $3d$  in  $\bar{p}$ -H(1s) collisions at  $\bar{p}$  energies from 1 to 200 keV, supplemented by still larger-Sturmian-basis one-center cross sections for ionization and excitation up to  $4f$  at overlapping energies from 5 to 16 000 keV. Detailed basis-convergence studies up to 200 keV show sensitivity in cross sections to be at most a few percent for ionization and the dominant excitation channels ( $2p$  and total excitation). Differences among individual excitation cross sections with various bases oscillate with energy within an absolute bound

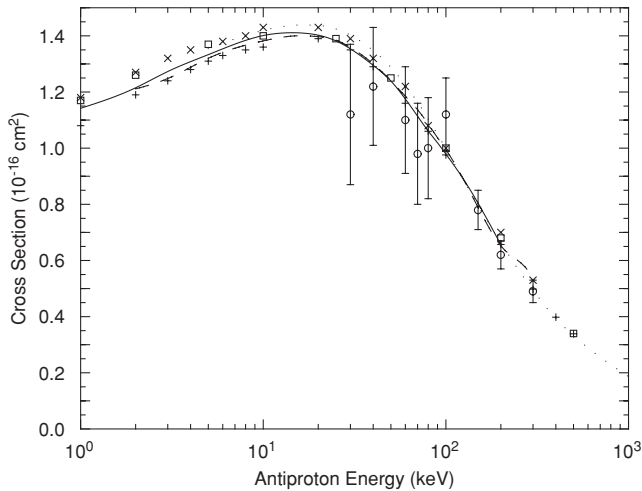


FIG. 6. Coupled-state and experimental cross sections for ionization in  $\bar{p}$ -H(1s) collisions. Solid curve, two-center 176-Sturmian (present result); dashed curve, two-center 220-Sturmian (present result); dotted curve, one-center 280-Sturmian (present result); crosses, two-center Gaussian-pseudostate (Toshima [7]); plus signs, one-center pseudostate (McGovern *et al.* [3]); squares, one-center Sturmian (Igarashi *et al.* [6]). Circles, experimental results of Knudsen *et al.* [21].

$\lesssim 2 \times 10^{-18} \text{cm}^2$ , such that the smaller channels, notably  $3s$  and  $3d$ , have sensitivities of up to 10–20%.

Differences with the coupled-state results of others are comparable to the above internal differences, and also typically oscillate with energy, at least for individual-state excitation. Different bases partition probability differently between ionization and excitation, such that the inelastic sum is rather insensitive to basis; recall Fig. 1. In most cases the present two-center ionization cross sections are below the present one-center cross sections and the one-center cross sections of others by a few percent, which may in part be attributed to the lack of  $g, h, \dots$  waves in the present calculations. However, the large-basis one-center ionization cross section of McGovern *et al.* [3] actually lies a few percent *below* the present two-center results. There is good agreement of most of the coupled-state results with the single available experimental cross section [21], which has large error bars.

There appear to be few *systematic* discrepancies among all the theoretical results exceeding about 10%: (1) At 2 keV the present two-center, 220-state  $3s$  cross section is below the theoretical cross sections cited in Sec. III A by 15–20%; this is consistent with the somewhat large basis sensitivity to  $n$  noted in Table I for this small cross section and low energies. (2) At 1 keV the present two-center, 164-state  $3d$  cross section

is below the cited theoretical cross sections by 10–20%, consistent with the somewhat large basis sensitivity to  $\ell$  noted in Table II for this small cross section and low energies. (3) At 200 keV, the numerical  $3d$  cross section of Sakimoto [9] is above the three present Sturmian cross sections by 20–30%. It should be emphasized that all of these possible systematic errors are in small cross sections.

For individual excitations to bound states at high energies, the present one-center cross sections monotonically approach corresponding first-Born cross sections: for excitation to within 0.1–0.2% by 16 MeV; for ionization the difference is 0.7%. Differences with corresponding one-center proton-impact cross sections also systematically become small at high energies.

The two-center  $s, p, d$  and  $s, p, d, f$  Sturmian bases apparently provide sufficient variational freedom with a limited number of  $\ell$  values (i.e.,  $\ell \leq 2$  or 3) to achieve accuracy comparable to one-center bases with significantly more  $\ell$  values. Further, as has been noted by Toshima [7] in his two-center Gaussian paper, only at energies below 1 keV is a two-center effect on the total ionization cross section pronounced. Even the present one-center  $s, p, d, f$  Sturmian bases are largely adequate for determining the integrated cross sections at the energies considered here.

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  - [12] For the one-center bases, a greater  $z$  range has sometimes been used, with <1% effect.
  - [13] The notation  $\rho = 0(0.3)3.6a_0$  indicates that the first interval is from 0 to  $3.6a_0$  in increments of  $0.3a_0$ , and similarly for the next intervals.
  - [14] There is a single exception: a relative error of 0.003% for the 220-state basis at 2 keV.
  - [15] There is also a 4.7% difference for  $3p$  at 3 keV.
  - [16] There is also a 3% difference for  $4f$  at 60 keV.
  - [17] There is a single exception: a 2.9% difference for excitation to all states at 3 keV.
  - [18] There is a 40% difference from the  $2s$  value of McGovern *et al.* [3] at 500 keV, but this difference may only be a reading error of their small *graphical* value.
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