Electron transfer, excitation, and ionization in collisions between protons and the ions He^+, Li^{2+}, Be^{3+}, B^{4+}, and C^{5+}

Thomas G. Winter

Department of Physics, Pennsylvania State University, Wilkes-Barre Campus, Lehman, Pennsylvania 18627, USA

(Received 2 February 2013; published 8 March 2013)

Coupled-state cross sections have been determined for electron transfer and excitation to individual states up to $3d$, as well as ionization, in collisions between protons and ground-state hydrogenic ions He^+, Li^{2+}, Be^{3+}, B^{4+}, and C^{5+} at intermediate and higher proton energies using two-center 120- and 281-Sturmian bases, extending previous smaller basis results by the author [Phys. Rev. A **35**, 3799 (1987)] at intermediate energies, and reexamining scaling rules with target nuclear charge Z.

DOI: 10.1103/PhysRevA.87.032704 PACS number(s): 34.70.+e, 34.50.Fa

I. INTRODUCTION

Electron transfer, excitation, and ionization in collisions between protons and hydrogenic ions is a fundamental class of atomic-collision processes. These three collision processes are nonresonant, with the electron tightly bound to the target nucleus—increasingly so as the target nuclear charge Z is increased—and the cross sections are generally small. At low projectile speeds, the electron cloud has time to adjust to the nuclear motion, and a coupled-state treatment of electron transfer with a small number of molecular states is appropriate. (A proton moving at the Bohr velocity $cZ/137$ has a kinetic energy of $25Z^2$ keV.) Such approaches were taken for $He^+(1s)$ targets more than 30 years ago by Winter *et al.* [1], Kimura and Thorson [2], and, somewhat more recently, Errea *et al.* [3] and Hose [4]. Coupled-state treatments of charge transfer in one-electron collisional systems have been reviewed by the author [5].

At low projectile energies, ionization is even less likely than capture, and so may be ignored. However, at intermediate energies on the order of $25Z^2$ keV, it begins to be an open channel, influencing capture; indeed, capture may be thought to proceed through continuum intermediate states, and the process becomes at least second order. Direct excitation of the target also becomes important, though having relatively little effect on capture. This persists to high energies, where all three processes may be treated perturbatively, capture to second order [6], and excitation and ionization to first order [7].

At intermediate energies, all three channels may be strongly coupled, particularly for lower-Z targets, and coupled-state approaches with explicit inclusion of ionization are needed. Such an approach—a coupled-Sturmian approach—was taken in 1987 by the author [8] for hydrogenic targets with $Z \leqslant 6$: He^+, Li^{2+}, Be^{3+}, B^{4+}, and C^{5+}, following earlier work for He^+ [9] and Li^{2+} [10] targets. Later work by Stodden *et al.* [11], Winter and Alston [12], and Winter and Winter [13] reported somewhat larger-basis Sturmian cross sections for He^+ targets, particularly at higher energies, and additional studies have been reported by the author [14,15] for C^{5+} targets.

However, these studies used somewhat small bases, and only reported cross sections for capture to the ground state, total capture, and ionization (except for a treatment of direct excitation of C^{5+} at MeV energies [15]). The present coupled-state study tests and improves the accuracy of these calculations with substantially larger bases, somewhat extends the energy range, and determines cross sections for direct excitation and excitation with capture. The extent to which high-energy scaling rules with Z [6,7] are valid at intermediate energies is also examined in greater detail.

The outline of the paper is as follows: The coupled-state method and numerical tests will be summarized in Sec. II. Cross sections will be presented in Sec. III and compared to results with other Sturmian bases, and to experimental as well as other theoretical results. The extent to which cross sections can be scaled to universal curves will be examined. Conclusions will be summarized in Sec. IV. Atomic units are used unless noted otherwise.

II. METHOD

A. Summary

Various bases are appropriate in coupled-state approaches for the presently considered processes, provided they include functions representing ionization as well as bound states. As in Refs. [8–15] and following Shakeshaft [16], the chosen Sturmian-basis functions on each center are just polynomials in the radial electronic variable r multiplied by a *fixed* exponential $e^{-\zeta r/[(\ell+1)]}$ (and a spherical harmonic), where $\zeta = Z = 2$–6 for target-centered functions and $\zeta = Z_A = 1$ for projectile-centered functions. The polynomials and therefore the Sturmians form a complete set. For hydrogen atoms and hydrogenic ions, the lowest electronic states $1s, 2p, 3d, \ldots$ of angular momenta $\ell = 0, 1, 2, \ldots$ are each represented exactly by a single Sturmian; states with positive Hamiltonian eigenvalues represent ionization [17,18].

The Sturmian basis on both centers is overly complete in the limit of a very large basis. In the present calculations with finite bases, problems of linear dependence did not arise. Such linear dependence, if it had occurred, would have manifested itself in various ways (particularly at the smallest impact parameters, at which there is the greatest overlap between functions on the two centers)—for example, in the failure of probability conservation or the inability to maintain a sufficiently small truncation error even with an extremely small time step.

In the semiclassical impact-parameter method, valid at intermediate and higher energies, the time-dependent electronic wave function is expanded in a basis of traveling atomic orbitals [19]. (The atomic basis functions on each nucleus are themselves obtained by diagonalizing the atomic

Hamiltonian in the Sturmian basis.) Substituting the expansion in the time-dependent Schrödinger equation and integrating over the electronic spatial coordinates yields a set of coupled first-order differential equations for the expansion coefficients $a_j(\rho,t)$, which, on integrating over the collision time t, yields the transition amplitudes to states labeled by j and the transition probabilities $P_j(\rho) = |a_j(\rho,t_{\max})|^2$ for a given impact parameter ρ. Integrating over ρ gives the transition cross sections Q_j.

B. Numerical tests

The present *numerical* error estimate in the last column of Tables I–V is the difference of the cross section summed over all channels (including the elastic channel) from $\pi\rho_{\max}^2$ (global probability conservation or unitarity [20]), and appears to be negligible. As in previous work [8–15,20], this error is partly due to the truncation-error limits e_1,e_2 in integrating the coupled equations over $z = vt$ and the number of integration points N_λ,N_μ and the limiting internuclear distance $R_{\max}$ in evaluating the charge-exchange matrix elements in spheroidal coordinates. For each target ion, the first was varied from $e_1,e_2 = 10^{-6,-4}$ to $10^{-7,-5}$ at three or more tabulated energies, negligibly affecting the cross sections in Tables I–V (changes being at most of the order of 10^{-22} cm^2). The second was varied from $N_\lambda,N_\mu = 36,80$ to 32, 40 at one or more lower tabulated energies and from 40, 96 to 36, 80 at two or more higher energies without changing any of the tabulated cross sections by more than one unit in the last reported digit. Lastly, the calculations have been redone at three or more tabulated energies using $R_{\max} = 80$ rather than 60, leaving unchanged the tabulated cross sections [21].

Three parameters—the ρ mesh, $\rho_{\max}$, and $z_{\max}$—relate only indirectly to the conservation of probability. The impact parameters used are generally $\rho = 0(0.0625)0.5(0.125)1(0.25)4$. For each target ion, the calculations were redone at three or more energies with the intervals $\delta\rho$ doubled, affecting the cross sections by at most one unit in the last tabulated place or 1% (except for B^{4+} ionization at 50 keV, for which it is 5%); considering that the error with Simpson's rule is of the order of $(\delta\rho)^4$, it may be supposed that the integration error with the smaller intervals is substantially <1%. Second, the calculations were redone for at least three tabulated energies with $\rho_{\max} = 6$ rather than 4. Only the cross sections for He^+ or Li^{2+} excitation to $2p$ or all states at higher energies are increased significantly (by up to 6% for He^+ excitation to $2p$ at 250 keV), with the tabulated values being with $\rho_{\max} = 6$. Finally, the calculations were redone at three tabulated energies with $z_{\max} = 1000$ rather than 500. Changes are, at most, one unit in the last reported digit, or 0.1%.

III. RESULTS

A. Basis sensitivity

1. Comparison with previous smaller Sturmian-basis results

Shown in Tables I–V are the present 120-Sturmian two-center cross sections. The basis is "symmetric": the Sturmian functions $\leqslant 13(s,p),7d,5f$ on each center, with the appropriate charge in the exponential ($Z_A = 1$ for projectile-centered functions, and $Z = 2$–6 for target-centered functions). Also shown are differences in the last digit(s) from available previous values by the author with smaller two-center Sturmian bases [8,14]. The present results extend to somewhat higher energies, and direct excitation was not previously reported, nor was capture into individual excited states. For each target ion, differences with the previously reported results are seen usually to oscillate with energy for ground-state and

TABLE I. Coupled-Sturmian cross sections (in units of 10^{-18} cm^2) vs proton energy E for electron transfer to excited states of H (upper half) and for ionization and direct excitation (lower half) in p-$He^+(1s)$ collisions using the basis $\leqslant 13(s,p),7d,5f$ on each center (120 states in all). When there are two numbers in parentheses, the first is the difference in the last digit(s) from the previous value [8] with 24–35 Sturmians. The second number in parentheses, or the single number in parentheses when there is only one, is the difference in the last digit(s) from the value using the basis $\leqslant 30(s,p,d,f)$ centered on the He nucleus and a single $1s$ function centered on the proton (281 states in all). For the latter basis, capture into all excited states has been estimated by an n^3 rule (implying a 20% contribution from excited states).

E(keV)	$1s$	$2s$	$3s$	$2p$	$3p$	$3d$	All	Error
17.5	9.4(3, 8)	0.1	0.0	0.1	0.0	0.0	9.8(2, −6)	0.004
31.25	22.0(6,22)	0.3	0.1	0.7	0.1	0.1	23.7(1, −1)	0.003
50	23.5(5,21)	0.6	0.1	1.1	0.3	0.0	26.3(−9, 5)	0.0007
75	16.8(−4,9)	0.9	0.2	0.6	0.2	0.0	19.4(−13, 2)	0.0005
100	10.8(0, 3)	0.9	0.2	0.3	0.1	0.0	12.7(−11, 1)	0.001
150	4.4(0, 0)	0.5	0.1	0.1	0.0	0.0	5.4(−4, 1)	0.002
250	0.9(0)	0.1	0.0	0.0	0.0	0.0	1.2(1)	0.005
E(keV)	Ionization	$2s$	$3s$	$2p$	$3p$	$3d$	All	
17.5	0.3(−2)	3.2(1)	0.1(0)	2.0(1)	0.3(0)	0.1(0)	6.2(3)	
31.25	2.5(11, −12)	6.4(4)	1.0(1)	4.0(6)	0.8(1)	0.2(0)	13.8(11)	
50	6.9(29, −13)	5.4(2)	1.2(1)	5.7(5)	0.9(1)	0.2(0)	15.7(15)	
75	11.6(42, 6)	3.9(2)	0.9(0)	6.9(0)	1.1(0)	0.2(0)	15.3(6)	
100	14.0(38, 16)	2.8(−1)	0.7(0)	7.4(−2)	1.3(0)	0.3(1)	14.8(1)	
150	14.8(40, 17)	1.9(0)	0.5(0)	7.8(1)	1.2(−1)	0.2(0)	13.5(−1)	
250	12.1(11)	1.1(0)	0.3(1)	6.5(−3)	1.2(0)	0.2(1)	11.0(0)	

TABLE II. Coupled-Sturmian cross sections (in units of 10^{-20} cm^2) vs proton energy E for electron transfer to excited states of H (upper half) and for ionization and direct excitation (lower half) in p-Li$^{2+}(1s)$ collisions using the basis $\leqslant 13(s,p),7d,5f$ on each center (120 states in all). When there are two numbers in parentheses, the first is the difference in the last digit(s) from the previous value [8] with 36–45 Sturmians. The second number in parentheses, or the single number in parentheses when there is only one, is the difference in the last digit(s) from the value using the basis $\leqslant 30(s,p,d,f)$ centered on the Li nucleus and a single $1s$ function centered on the proton (281 states in all). For the latter basis, capture into all excited states has been estimated by an n^3 rule.

E(keV)	$1s$	$2s$	$3s$	$2p$	$3p$	$3d$	All	Error
17.5	2.2(−1, 2)	0.0	0.0	0.0	0.0	0.0	2.3(−4, −1)	0.004
30	26(0, 2)	1	0	0	0	0.0	28(0, −1)	0.003
50	96(6, 9)	2	1	3	1	0.4	106(−2, 2)	0.003
100	173(−2,17)	7	1	10	3	0.5	201(−6,14)	0.04
125	163(2,14)	9	2	9	3	0.2	192(−2,13)	0.003
200	103(8, 9)	8	2	2	1	0	120(2, 7)	0.07
400	22(2)	2	1	0	0	0	26(1)	0.09
600	5(0)	1	0	0	0	0	7(0)	0.03
1000	0.7(0)	0	0	0	0	0	0.8(−1)	0.02
E(keV)	Ionization	$2s$	$3s$	$2p$	$3p$	$3d$	All	
17.5	0.6(−1)	6.0(0)	0.4(1)	5.4(3)	0.3(0)	0.14(−5)	12.4(0)	
30	5(0, −1)	62(4)	3(0)	23(2)	4(0)	1(0)	98(5)	
50	34(7, −3)	133(8)	21(3)	73(4)	11(2)	2(0)	262(17)	
100	172(33, 8)	122(3)	30(2)	153(3)	25(2)	4(0)	388(14)	
125	230(35,16)	102(1)	27(3)	169(3)	28(1)	4(0)	384(9)	
200	313(28,29)	66(1)	15(−1)	181(0)	32(1)	5(1)	348(4)	
400	283(22)	32(1)	6(−1)	159(−3)	27(−1)	3(0)	264(−3)	
600	208(−1)	20(0)	5(1)	135(−5)	24(0)	2(0)	215(−4)	
1000	136(−9)	11(−1)	2(0)	110(0)	19(0)	1(0)	164(0)	

total capture. On the other hand, the present ionization cross section for a given target ion is always above the previous cross section, or always below, independent of energy.

Averaged over energy, the *percent* differences for the most part grow with increasing target nuclear charge Z for both capture to the ground-state and total capture, but not for ionization. For ground-state and total capture, the largest average differences (15% and 22%, respectively) are for $Z = 6$ (C^{5+} targets), for which cross sections are the smallest. On the other hand, the largest average difference for ionization (35%) is for $Z = 2$, for which not only are the cross sections somewhat small, but also a smaller basis was used; the average

TABLE III. Coupled-Sturmian cross sections (in units of 10^{-20} cm^2) vs proton energy E for electron transfer to excited states of H (upper half) and for ionization and direct excitation (lower half) in p-Be$^{3+}(1s)$ collisions using the basis $\leqslant 13(s,p),7d,5f$ on each center (120 states in all). When there are two numbers in parentheses, the first is the difference in the last digit(s) from the previous value [8] with 45 Sturmians. The second number in parentheses, or the single number in parentheses when there is only one, is the difference in the last digit(s) from values using the basis $\leqslant 30(s,p,d,f)$ centered on the Be nucleus and a single $1s$ function centered on the proton (281 states in all). For the latter basis, capture into all excited states has been estimated by an n^3 rule.

E(keV)	$1s$	$2s$	$3s$	$2p$	$3p$	$3d$	All	Error
50	2.9(−2, 1)	0.14	0.02	0.03	0.01	0.00	3.2(−5, −2)	0.0004
100	17.2(29,15)	0.4	0.1	0.9	0.2	0.1	19.6(3, 8)	0.01
150	25.4(15,29)	1.1	0.2	1.1	0.4	0.05	29.2(6,22)	0.02
200	24.8(−16,19)	1.7	0.4	1.4	0.4	0.04	29.8(−1,22)	0.007
400	12.5(17,12)	1.3	0.3	0.3	0.1	0.0	14.9(17,13)	0.01
1000	1.0(0)	0.1	0.0	0.0	0.0	0.0	1.3(1)	0.06
E(keV)	Ionization	$2s$	$3s$	$2p$	$3p$	$3d$	All	
50	2.2(4, 0)	21.5(5)	1.9(1)	6.9(1)	1.0(2)	0.3(1)	32.9(6)	
100	20.9(28,22)	41.2(11)	8.6(6)	33.2(3)	4.5(2)	0.8(2)	98.0(15)	
150	47.7(59,26)	38.1(7)	9.0(3)	49.8(8)	7.5(−1)	1.0(0)	122(3)	
200	71.0(96,43)	31.9(3)	7.9(4)	57.3(8)	9.9(5)	1.4(2)	125(2)	
400	99(1, 5)	17.6(6)	3.8(−1)	59.8(−5)	10.2(−4)	1.3(1)	108(1)	
1000	69.1(12)	6.2(−3)	1.3(−1)	46.4(0)	8.1(0)	0.7(0)	72.0(−3)	

TABLE IV. Coupled-Sturmian cross sections (in units of 10^{-20} cm^2) vs proton energy E for electron transfer to excited states of H (upper half) and for ionization and direct excitation (lower half) in p-B$^{4+}(1s)$ collisions using the basis $\leqslant 13(s,p),7d,5f$ on each center (120 states in all). When there are two numbers in parentheses, the first is the difference in the last digit(s) from the previous value [8] with 55–60 Sturmians. The second number in parentheses, or the single number in parentheses when there is only one, is the difference in the last digit(s) from values using the basis $\leqslant 30(s,p,d,f)$ centered on the B nucleus and a single $1s$ function centered on the proton (281 states in all). For the latter basis, capture into all excited states has been estimated by an n^3 rule.

E(keV)	$1s$	$2s$	$3s$	$2p$	$3p$	$3d$	All	Error
50	0.09(0)	0.01	0.00	0.00	0.00	0.00	0.12(2)	0.0007
75	0.6(−1,0)	0.0	0.0	0.0	0.0	0.0	0.7(−2,0)	0.003
100	1.4(0,0)	0.1	0.0	0.1	0.0	0.0	1.7(−3,0)	0.001
200	5.6(10,9)	0.2	0.1	0.3	0.1	0.0	6.6(11,9)	0.0004
300	5.6(2,4)	0.4	0.1	0.3	0.1	0.0	6.8(5,5)	0.0004
400	4.7(−3,2)	0.4	0.1	0.2	0.1	0.0	5.7(−2,3)	0.0005
600	3.0(1,3)	0.3	0.1	0.0	0.0	0.0	3.5(−1,3)	0.0006
937.5	1.1(0)	0.1	0.0	0.0	0.0	0.0	1.3(0)	0.01
1500	0.3(0)	0.0	0.0	0.0	0.0	0.0	0.4(1)	0.03
E(keV)	Ionization	$2s$	$3s$	$2p$	$3p$	$3d$	All	
50	0.24(−2)	3.46(−2)	0.17(−1)	0.64(−1)	0.11(2)	0.04(1)	4.54(−4)	
75	1.1(0, 1)	8.8(2)	1.0(0)	3.1(0)	0.3(0)	0.1(0)	13.8(0)	
100	2.9(−2, 4)	12.6(3)	2.0(0)	6.9(0)	0.7(0)	0.1(0)	23.9(0)	
200	16(−1, 0)	14.9(2)	3.6(3)	19.3(2)	3.0(1)	0.4(1)	46.7(5)	
300	28(−2, 1)	12.3(1)	3.0(1)	24.3(4)	3.9(−1)	0.4(−1)	51.0(8)	
400	35(−2, 1)	10.1(3)	2.3(0)	25.6(1)	4.3(−1)	0.5(0)	49.7(5)	
600	39(−5, 1)	6.9(1)	1.7(2)	24.9(−5)	4.6(1)	0.5(0)	44.8(1)	
937.5	38(−3, 2)	4.2(−2)	0.9(−1)	23.1(0)	4.1(0)	0.4(0)	37.8(−1)	
1500	32.5(43)	2.7(0)	0.6(0)	20.2(7)	3.2(−2)	0.3(0)	31.2(9)	

difference of the present cross sections from the 51-Sturmian values of Stodden *et al*. [11,22] is only 13%.

Averaged over both energy and nuclear charge, the present 120-Sturmian results differ by 8%, 10%, and 16% from the

TABLE V. Coupled-Sturmian cross sections (in units of 10^{-20} cm^2) vs proton energy E for electron transfer to excited states of H (upper half) and for ionization and direct excitation (lower half) in p-C$^{5+}(1s)$ collisions using the basis $\leqslant 13(s,p),7d,5f$ on each center (120 states in all). When there are two numbers in parentheses, the first is the difference in the last digit(s) from the previous value [14] with 60 Sturmians. The second number in parentheses, or the single number in parentheses when there is only one, is the difference in the last digit(s) from values using the basis $\leqslant 30(s,p,d,f)$ centered on the C nucleus and a single $1s$ function centered on the proton (281 states in all). For the latter basis, capture into all excited states has been estimated by an n^3 rule.

E(keV)	$1s$	$2s$	$3s$	$2p$	$3p$	$3d$	All	Error
125	0.27(−5, −1)	0.01	0.01	0.01	0.00	0.00	0.33(−11,0)	0.002
250	1.4(3, 1)	0.1	0.0	0.1	0.0	0.0	1.8(4,3)	0.003
375	1.8(2, 2)	0.1	0.0	0.1	0.0	0.0	2.1(2,2)	0.01
500	1.4(0, 0)	0.1	0.0	0.1	0.0	0.0	1.8(1,1)	0.002
625	1.2(0, 0)	0.1	0.0	0.1	0.0	0.0	1.5(0,1)	0.001
750	1.1(0, 1)	0.1	0.0	0.0	0.0	0.0	1.2(−2,0)	0.0005
875	0.8(−3, 0)	0.1	0.0	0.0	0.0	0.0	1.0(−3,1)	0.001
1000	0.6(−2, 0)	0.1	0.0	0.0	0.0	0.0	0.7(−4,0)	0.003
E(keV)	Ionization	$2s$	$3s$	$2p$	$3p$	$3d$	All	
125	1.08(−12,17)	5.11(9)	0.79(2)	2.68(−1)	0.24(0)	0.05(1)	9.44(−5)	
250	6.1(−8, 1)	6.8(1)	1.6(1)	8.6(1)	1.2(0)	0.1(0)	20.7(2)	
375	11.6(−10, 1)	6.0(1)	1.4(0)	11.3(1)	1.8(−1)	0.2(0)	23.9(3)	
500	15.7(−15, 6)	5.0(1)	1.2(1)	12.3(0)	2.2(1)	0.2(0)	24.0(1)	
625	17.8(−24, 7)	4.2(0)	1.0(1)	12.5(−1)	2.3(1)	0.2(0)	23.4(2)	
750	19.0(−24, 9)	3.5(−1)	0.8(0)	12.5(−1)	2.2(0)	0.2(0)	22.5(2)	
875	19.6(−23,13)	3.0(−1)	0.7(0)	12.4(0)	2.2(0)	0.2(0)	21.5(1)	
1000	19.9(−17,17)	2.6(−1)	0.6(0)	12.2(1)	2.2(1)	0.2(0)	20.7(2)	
2000	16.4(23)	1.5(1)	0.3(0)	9.7(−1)	1.8(1)	0.2(1)	15.5(3)	

previous smaller basis results for capture to the ground state, total capture, and ionization, respectively.

2. Comparison with present 100-Sturmian results

Prior to calculating cross sections with the 120-Sturmian basis, the author used a similar, but somewhat smaller, symmetric 100-Sturmian basis: the Sturmians $\leqslant 12(s,p),6d,4f$ on each center. Differences (not shown in the tables) between the 120- and 100-Sturmian cross sections for capture to the ground state, total capture, and ionization, as well as total direct excitation, are usually not more than one unit in the last digit of the cross sections in Tables I–V. Only for a few small $Z \geqslant 4$ capture cross sections do differences of more than one unit also exceed 6% [23]. Differences are substantially smaller than those between 120-Sturmian and the previously reported, smaller basis results, and suggest convergence is setting in.

The 120-Sturmian cross sections for excitation (direct or with transfer) to individual excited states have also been compared to results with the 100-Sturmian basis. For He^+ (i.e., $Z = 2$) targets, no difference exceeds one unit in the last reported cross-section digit in Table I. For capture into excited states from higher-Z targets, only for Be^{3+} ($Z = 4$) targets (Table III) at 100–200 keV do some differences exceed one unit [24]. For direct excitation of higher-Z targets, differences exceeding one unit in the last reported digit are, for the most part, small percentages [25].

3. Comparison with present 281-Sturmian results

Also shown in Tables I–V with the present 120-Sturmian, two-center cross sections are differences in the last digit(s) from present values using a very asymmetric 281-Sturmian basis (280 Sturmians centered on the target nucleus and a single $1s$ function centered on the proton). Differences tend to oscillate somewhat with projectile energy (though not always to the extent of changing sign). There are large differences for ionization of He^+ and Li^{2+} at low energies, probably reflecting the importance of charge transfer to the continuum, and possibly also ionization from the saddle point of the electronic potential [26–28], and so the smaller (symmetric 120-Sturmian) basis would be expected to be superior there. On the other hand, there are large differences for electron capture from B^{4+} and C^{5+}, probably due to the increasing dominance of second-order processes at high energies and the need to include a large number of intermediate states, as with the 281-Sturmian basis.

Averaged over energy, the *percent* differences grow somewhat with Z for capture to the ground state and to all states. For ionization, $2p$ excitation, and total excitation, the reverse is true: percent differences generally decrease somewhat with increasing Z. This is to be expected, since ionization and excitation become more important than capture at higher Z, and hence less sensitive to basis if the important channels centered on the target nucleus are represented.

Averaged over both energy and nuclear charge, the 120- and 281-Sturmian results differ by 7–8% for capture to the ground state and total capture, 10% for ionization, and 2% for $2p$ and total excitation. For $2s$ excitation, the average difference is 3%. The $n = 3$ excitation cross sections are smaller, and so the basis sensitivity would be expected to be greater; this is indeed the case in percentage terms, although the absolute sensitivities are of the same order as for $n = 2$ states.

B. Comparison with other theoretical and with experimental results

1. p-He$^+$ collisions

The 120-Sturmian cross section for capture to all states of H in intermediate-energy p-$He^+(1s)$ collisions is shown in Fig. 1 together with other coupled-state results: the norm-optimized, molecular-state result of Errea *et al.* [3], the two-center, atomic-pseudostate result of Bransden *et al.* [29], and the author's result with a three-center, atomic-state basis [28]. The agreement among the norm-optimized, two-center-pseudostate, three-center, and Sturmian results is within 5% at a center-of-mass energy of 40 keV (corresponding to a proton energy of 50 keV) near the cross section's peak. On the other hand, the 45-molecular-state cross section of Hose [4] (not shown) is about 40% lower there. Also not shown is the earlier 10-molecular-state cross section of Winter *et al.* [1], which only goes up to 14 keV, which is the lowest energy of the present calculation. At this energy, the result of Hose is about 5% below that of Winter *et al.*, which is itself about 35% below the present 120-Sturmian value. Both molecular-state bases omit the molecular continuum.

Coupled-state results for total capture are also shown in Fig. 1 along with the experimental results of Peart *et al.* [30] and Watts *et al.* [31], both with total estimated error bars. Agreement between the experimental and theoretical results is

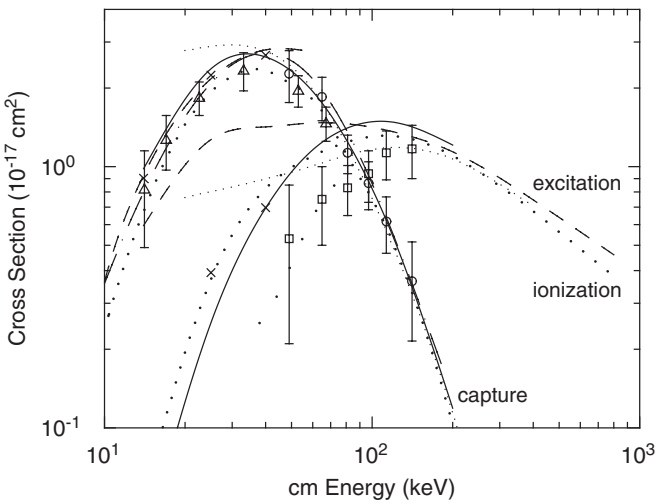

FIG. 1. Cross sections for electron capture and direct excitation to all states, as well as ionization, in p-$He^+(1s)$ collisions. Capture, coupled-state results: 120-Sturmian, present result (solid line); norm-optimized molecular [3] (dashed line); three-center atomic [28] (crosses); two-center atomic-plus-pseudo [29] (dash-dotted line); one-and-a-half-center [32] (close-dotted line). Capture, numerical result: Tong *et al.* [33] (dotted line). Capture, experimental results: Peart *et al.* [30] (triangles); Watts *et al.* [31] (circles). Excitation, coupled-state result: 281-Sturmian (dashed curve). Ionization, coupled-state results: 281-Sturmian (dotted curve); 120-Sturmian (solid curve); three-center atomic [28] (crosses); one-and-a-half-center [32] (close-dotted line). Ionization, experimental results: Peart *et al.* [30] (widely-spaced dotted line); Watts *et al.* [31] (squares).

generally very good. The one-and-a-half-center cross section of Reading *et al*. [32] lies above the other theoretical results and experiment below 40 keV; at higher energies, the agreement is excellent, as expected with a large, predominantly target-centered basis. Shown also is the numerical cross section of Tong *et al*. [33], which agrees with the experimental and with most of the coupled-state cross sections in the displayed range of energies.

Shown also in Fig. 1 are the coupled-Sturmian cross sections for total excitation and ionization. The 120-Sturmian cross section for ionization at lower energies (to be preferred over the 281-Sturmian cross section there) lies somewhat above the large total error bars of Watts *et al*. [31]; at higher energies, the (preferred) 281-Sturmian cross section lies within the error bars. The error bars on the measurements of Peart *et al*. [30] are not given, but may be similarly large, in view of the procedure of obtaining the ionization cross section by subtracting the capture cross section from the total He^{2+} production cross section. The author's result with a three-center basis [28] agrees with the 120-Sturmian cross section at 40 keV, but appears too high at 25 keV, though agreeing there with the 281-Sturmian value. The one-and-a-half-center cross section of Reading *et al*. [32] agrees well at intermediate energies, but is much too high at 20 keV, probably due to their including the important 1*s* capture channel only perturbatively.

2. *p*-Li^{2+} collisions

Both 120- and 281-Sturmian cross sections for capture to all states of H in intermediate-energy *p*-$Li^{2+}(1s)$ collisions are shown in Fig. 2, as well as for total direct excitation and ionization. With the exception of ionization at lower energies, the two sets of cross sections are hard to distinguish on the scale of this graph. Also shown are the one-and-a-half-center cross sections of Ford *et al*. [34] both for capture and ionization, with their data points at 50, 100, and 200 keV being joined by smooth curves. There is excellent agreement with the coupled-Sturmian results, except that their ionization cross section at 50 keV is somewhat too high, probably, as for He^+, because of their treating the important 1*s* capture channel only perturbatively.

C. Overall variations

Cross sections for electron transfer to all states, direct excitation to all states, and ionization are graphed in Fig. 3 for all target ions (i.e., $Z = 2$–6). There is an enormous but systematic variation with both energy and target charge: Capture dominates excitation and ionization at lower energies for lower-Z targets, whereas for higher-Z targets, excitation and ionization dominate at all displayed energies. The relation between excitation and ionization is roughly independent of Z. For smaller Z at lower energies, capture is important, and ionization is a two-center process; thus, where there is a significant difference between results with the symmetric 120-Sturmian basis and the larger, 281-Sturmian asymmetric basis, results with the former are to be preferred. At high energies, the opposite is true.

1. Overall scaling

The systematic variations in Fig. 3, in fact, reflect scaling rules. The same cross sections are shown in Fig. 4 multiplied by Z^7 for electron transfer and Z^4 for excitation and ionization (these scalings being valid in the high-energy limit [6,7]), with the proton energies divided by $Z^2 \times 25$ keV (the square of the proton speed v in units of the Bohr velocity of the target electron, with this Bohr velocity being proportional to Z). Now, for capture, unlike for ionization and direct excitation, the

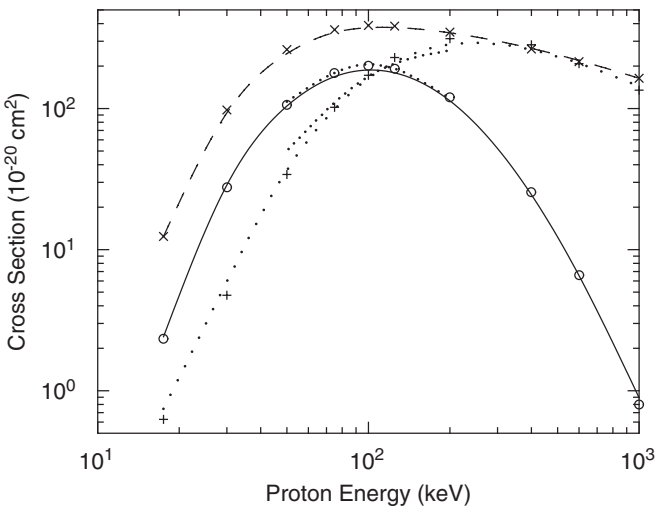

FIG. 2. Coupled-Sturmian two-center cross sections for electron transfer to all states (solid curve and circles), excitation (dashed curve and crosses), and ionization (dotted curve and plus signs) in collisions between protons and $Li^{2+}(1s)$ ions. The symbols are with a symmetric 120-Sturmian basis, while the curves are with an asymmetric 281-Sturmian basis. Also shown for capture and ionization as close-dotted lines are the one-and-a-half-center results of Ford *et al*. [32]. The latter two capture results assume an n^3 rule to account for excited states.

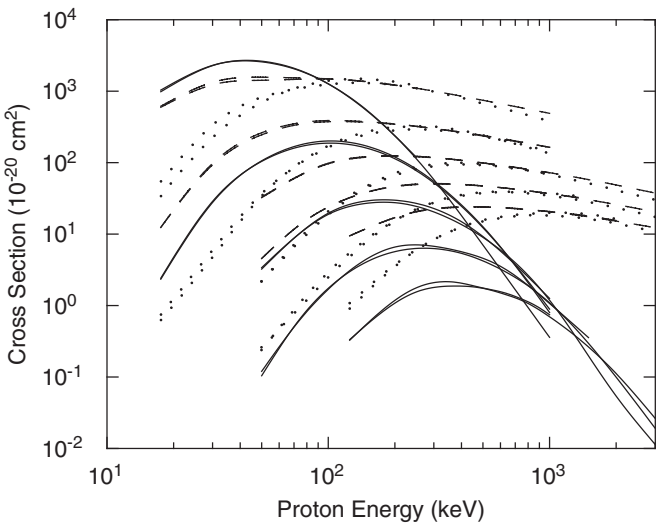

FIG. 3. Coupled-Sturmian two-center cross sections for electron transfer to all states (solid curves), excitation (dashed curves), and ionization (dotted curves) in collisions between protons and hydrogenic ions. The curves of each type, from top to bottom on the left, are for He^+, Li^{2+}, Be^{3+}, B^{4+}, and C^{5+} ions. The results here are with both the symmetric 120-Sturmian and asymmetric 281-Sturmian bases to summarize the range of basis sensitivity.

projectile-energy dependence of the cross section is contained not only in terms depending on the proton speed relative to the orbital speed of the target electron, but also in terms depending on the proton speed relative to the orbital speed of the captured electron; thus, in the present case of proton projectiles with $Z_A = 1$, even at higher energies the simple energy scaling with $v^2 = E/(Z^2 \times 25\ \text{keV})$ would only be expected to be valid to the order of $(Z_A/Z)^2$; this complication holds not only in second-order perturbation theory, which is required for capture at high energies [6], but also in first-order perturbation theory [35].

It is seen in Fig. 4 that the electron-transfer curves, while distinct at lower energies, do, nonetheless, appear to coalesce into a single curve at higher energies. Likewise, the excitation curves coalesce into one curve, as do the ionization curves. At most of the displayed energies, the transfer curves rise monotonically with Z, and at the lower energies, but not at their peaks, the excitation and ionization curves do as well. The greater departure from simple scaling is for smaller Z, where (at least down to peak energies) cross sections are larger, and low-order perturbation theory, on which the scaling rules are based, is less valid. With the 281-Sturmian basis, the scaled *peak* capture cross section increases smoothly from 3.4×10^{-15} cm^2 to 5.3×10^{-15} cm^2 as Z increases from 2 to 6, with the range being 4.3×10^{-15} cm$^2 \pm 20\%$ at $v^2 \approx 0.4$. The behavior is similar with the 120-Sturmian basis, but then the peak cross section is, on average, 9% higher, in part due to the greater contribution from excited states, which for the 281-Sturmian basis was assumed to be 20% in the absence

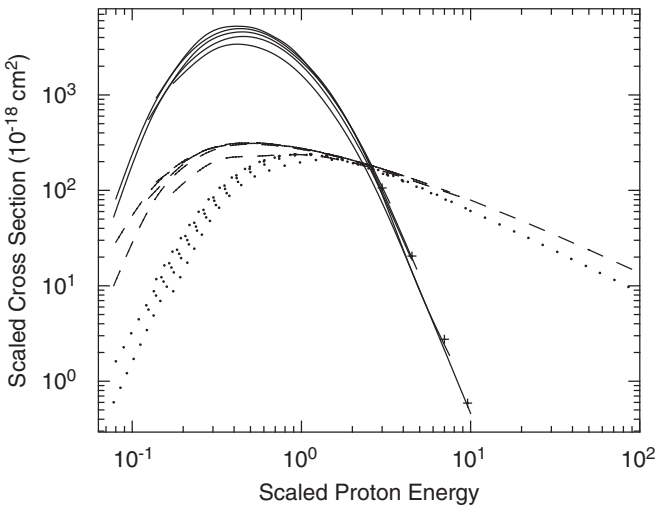

FIG. 4. Scaled coupled-Sturmian two-center cross sections for electron transfer to all states (solid curves), excitation (dashed curves), and ionization (dotted curves) in collisions between protons and hydrogenic ions vs scaled energy $E/(Z^2 \times 25\ \text{keV}) = v^2$. For capture, the curves, from bottom to top at the peak, are for He^+, Li^{2+}, Be^{3+}, B^{4+}, and C^{5+} ions. For excitation and ionization, the curves, from bottom to top at the left, are for He^+, Li^{2+}, Be^{3+}, B^{4+}, and C^{5+} ions. For clarity, the results are shown only with the asymmetric 281-Sturmian basis. The ionization and excitation curves for $v^2 > 10$ are scaled first Born cross sections. The + signs for $v^2 \geqslant 3$ are scaled cross sections using the impulse version of the strong-potential Born approximation for electron transfer to all states in p-He^+ collisions [12].

of open excited-state capture channels. Except for $Z = 2$, the scaled peak cross sections for total excitation and for ionization are within narrow ranges: 3.1×10^{-16} cm$^2 \pm 2\%$ at $v^2 \approx 0.51 \pm 0.01$ (close in *location* to the Born peak at $v^2 = 0.56$, $v \approx 3/4$) and 2.4×10^{-16} cm$^2 \pm 1\%$ at $v^2 \approx 1.0 \pm 0.1$, respectively, using the 281-Sturmian basis; for excitation, the 120-Sturmian peak cross section agrees, but there is a somewhat larger spread in the 120-Sturmian peak ionization cross section (2.5×10^{-16} cm$^2 \pm 4\%$ at $v^2 \approx 1.1 \pm 0.1$), with the 281-Sturmian ionization cross sections probably being more reliable there and at higher energies [36].

In summary, both for excitation and ionization, convergence toward Z-independent values sets in rapidly as the energy is increased (though less so for $Z = 2$). Therefore, beyond $v^2 = 10$, the cross sections displayed in Fig. 4 are first Born values. At $v^2 = 10$ for $Z = 2$, they differ from the 281-coupled-Sturmian values by <0.5% for ionization and 0.8% for total excitation (the latter decreasing to 0.1% by $v^2 = 50$). For consistency with the coupled-state approach, only partial waves $\ell \leqslant 3$ are included in the Born results; the $\ell = 4,5$ waves contribute 3–4% to the ionization cross section. For excitation, only Born cross sections through $4d$ were explicitly calculated; contributions from more highly excited states (≈7%), which are included, were assumed to be the same as in the coupled-state calculations.

Capture negligibly affects excitation and ionization at high energies: By $v^2 = 10$, 280-Sturmian cross sections (i.e., without the $1s$ capture channel) for ionization and total excitation of He^+ differ from 281-Sturmian values by $\leqslant 0.1\%$.

The scaled capture cross sections themselves also appear to converge toward a universal curve at higher energies; note the close agreement in Fig. 4 with the impulse version of the strong-potential Born approximation for p-He^+ collisions determined by Winter and Alston [12].

2. *Scaling for direct excitation to individual states*

Shown in Fig. 5 are scaled 281-Sturmian cross sections versus scaled proton energy for direct excitation of the $2p$ and $3p$ states and in Fig. 6 for direct excitation of the $2s$ and $3s$ states for all target ions from $Z = 2$ to 6. Cross sections have again been multiplied by Z^4 to test the scaling for individual states, valid in the high-energy limit. Except for $Z = 2$, all np cross sections peak in the narrow range $v^2 \approx 0.85 \pm 0.15$, in magnitudes 1.6×10^{-16} cm$^2 \pm 6\%$ and 2.7×10^{-17} cm$^2 \pm 6\%$ for $n = 2,3$, respectively. Similarly, except for $Z = 2$, all ns cross sections peak in a narrow range $v^2 \approx 0.32 \pm 0.05$, in magnitudes 1.0×10^{-16} cm$^2 \pm 10\%$ and 2.1×10^{-17} cm$^2 \pm 10\%$ for $n = 2,3$, respectively. Thus s excitation peaks at a lower speed ($v \approx 0.5$) than p excitation ($v \approx 0.9$), and the overall excitation peaks somewhere in between—at $v \approx 3/4$, as noted previously. However, the order with respect to Z is inverted: scaled s cross sections *decrease* with increasing Z for $Z > 2$ at peak and higher energies.

Also shown in Fig. 5 are first Born np cross sections. For $n = 2$ as well as 3, the location of the Sturmian cross section's peak moves in monotonically from $v^2 \approx 1.4$ to 0.7 (v decreasing from 1.2 to about 0.8), approaching the Born position, as Z increases from 2 to 6, and the height of the peak grows smoothly by 30%, approaching the Born height to

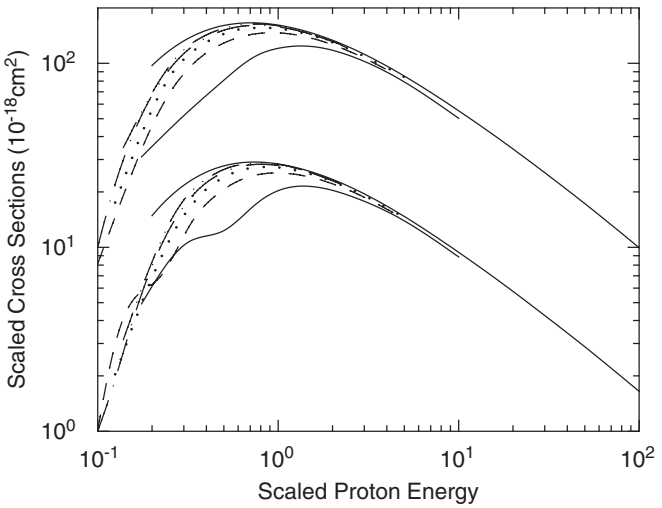

FIG. 5. Scaled cross sections for direct excitation to the $2p$ state (upper set of curves) and $3p$ state (lower set of curves) in collisions between protons and hydrogenic ions vs scaled energy $E/(Z^2 \times 25\ \text{keV}) = v^2$. The solid, dashed, dotted, dash-dotted, and dash-double-dotted curves are for He^+, Li^{2+}, Be^{3+}, B^{4+}, and C^{5+} ions, respectively. For clarity, the results are shown only with the asymmetric 281-Sturmian basis; results with the 120-Sturmian basis are similar. The curves for $v^2 > 10$ are first Born cross sections; they are also extended to lower energies.

within 1%. The curves for $3p$ are similarly shaped and in the same positions as the corresponding curves for $2p$, but are a factor of 5.7 lower. The structure in the $3p$ He^+ cross section at $v^2 \approx 0.6$ appears as well to some extent in the 120-Sturmian cross section (not shown), and thus is probably real, although this small cross section is sensitive to the choice of basis.

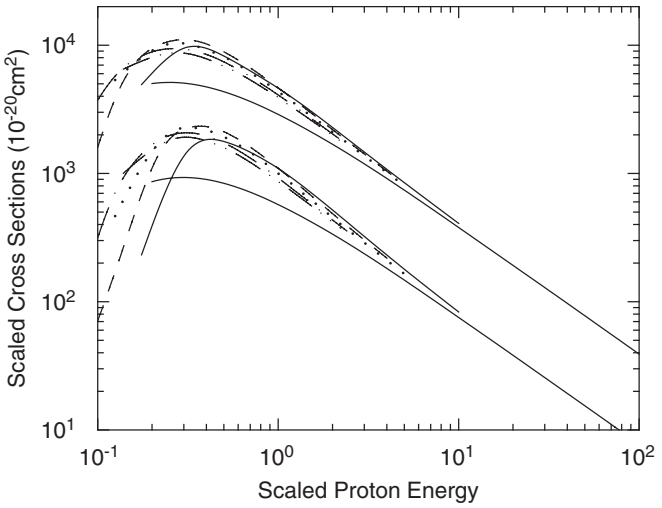

FIG. 6. Scaled cross sections for direct excitation to the $2s$ state (upper set of curves) and $3s$ state (lower set of curves) in collisions between protons and hydrogenic ions vs scaled energy $E/(Z^2 \times 25\ \text{keV}) = v^2$. The solid, dashed, dotted, dash-dotted, and dash-double-dotted curves are for He^+, Li^{2+}, Be^{3+}, B^{4+}, and C^{5+} ions, respectively. For clarity, the results are shown only with the asymmetric 281-Sturmian basis; results with the 120-Sturmian basis are similar. The curves for $v^2 > 10$ are first Born cross sections; they are also extended to lower energies.

The first Born cross sections for ns have also been extended to lower energies where the s state cross sections peak. However, it is clear in Fig. 6 that the situation for these smaller cross sections is more complicated than for the dominant p cross sections; only for $Z > 2$ does the ns coupled-state cross section monotonically approach the first Born cross section (from above) as Z is increased up to six, and it remains distant from it.

3. Scaling for electron capture to individual states

Shown in Fig. 7 are scaled 120-Sturmian cross sections versus scaled proton energy for electron capture to the $1s$ state of H for all target ions from $Z = 2$ to 6. Cross sections have here been multiplied by Z^7 to test this scaling for individual states, valid in the high-energy limit. For $1s$ capture, cross sections with 281 Sturmians are also determined, and are slightly lower for each Z than the 120-Sturmian result, but preserve the monotonically increasing peak height with respect to increasing Z.

For capture to excited states, 120-Sturmian results have instead been compared with smaller-basis 100-Sturmian values. For capture from He^+ to the $2s$ and $3s$ states, the 120-Sturmian cross sections agree fairly closely with 100-Sturmian curves (not shown). However, for capture to $2s,3s$ from higher-Z targets, cross sections with the two bases differ significantly, and are omitted from the graph. Small cross sections are more sensitive to basis size and numerical parameters; recall that in Tables I–V excited capture cross sections are generally only tabulated to one digit. Qualitatively, the $2s,3s$ peak cross sections increase monotonically with Z, as for $1s$.

The scaled $3p$ capture curve shown in Fig. 8 for He^+ is about a factor of four below the corresponding $2p$ curves, and slightly to the right. Only these two curves, and the $2p$ curve

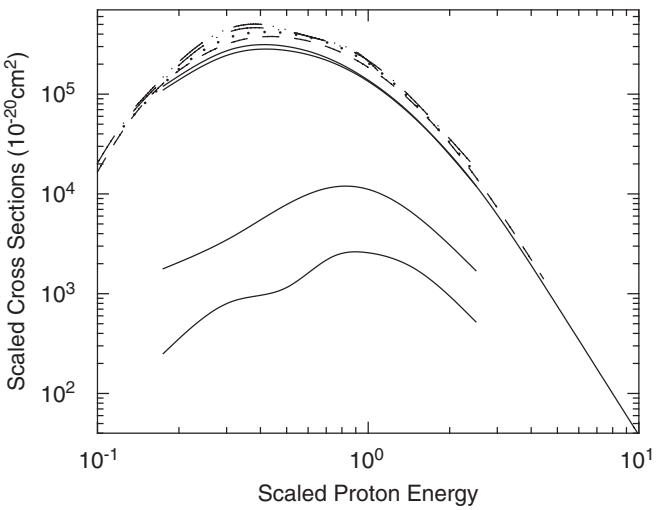

FIG. 7. Scaled 120-Sturmian cross sections for electron capture to the $1s$ state in collisions between protons and hydrogenic ions vs scaled energy $E/(Z^2 \times 25\ \text{keV}) = v^2$. The solid, dashed, dotted, dash-dotted, and dash-double-dotted curves are for He^+, Li^{2+}, Be^{3+}, B^{4+}, and C^{5+} ions, respectively. For $1s$, results are shown also with the asymmetric 281-Sturmian basis, but for He^+ only. The next-to-lowest and lowest solid curves are for capture from He^+ to $2s$ and $3s$, respectively, with the 120-Sturmian basis.

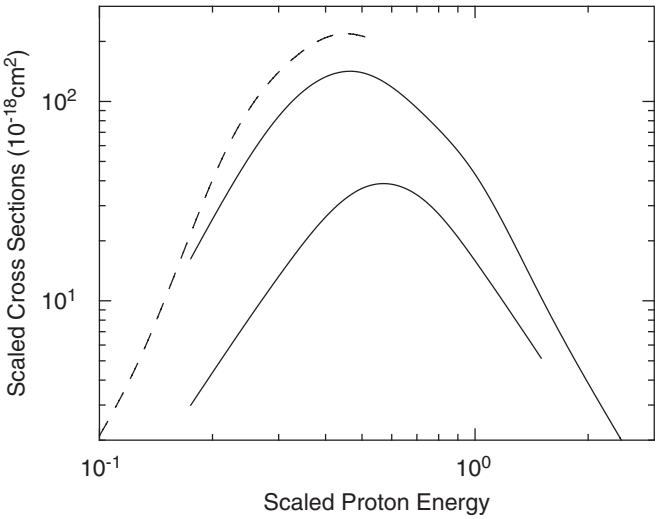

FIG. 8. Scaled 120-Sturmian cross sections for electron capture to the $2p$ state (upper two curves) and $3p$ state (lowest curve) in collisions between protons and hydrogenic ions vs scaled energy $E/(Z^2 \times 25\ \text{keV}) = v^2$. The solid and dashed curves are for He^+ and Li^{2+} ions, respectively.

for Li^{2+}, agree fairly closely with corresponding curves with the 100-Sturmian basis (not shown); curves for other collision processes are therefore omitted here.

IV. CONCLUSION

Coupled-state cross sections have been determined for electron transfer, excitation, and ionization in intermediate-energy collisions between protons and the first five hydrogenic ions using two bases: a 120-Sturmian basis with an equal number of Sturmians on each center, and a 281-Sturmian basis with all but one Sturmian centered on the target nucleus. Differences typically oscillate with energy. Averaged over energies and targets, these two sets of results differ by 7–8% for ground-state and total capture, 2–3% for $2s,2p$ and total excitation, and 10% for ionization. [With the 281-Sturmian basis, an n^3 (20%) rule has been used for capture to excited states.] Cross sections have also been compared to unpublished results with a 100-Sturmian basis having an equal number of Sturmians on each center. Differences of 120-Sturmian results from these results are generally smaller than differences from previously published results with 24 to 60 Sturmians, suggesting further that basis convergence is setting in. For ionization and capture from smaller-Z targets at lower energies, the collision processes likely have a two-center character, and the 120-Sturmian basis is probably superior to the 281-Sturmian basis, which is a conclusion supported by limited experimental results for ionization from He^+. At higher energies—certainly at energies above the cross sections' peaks—the 281-Sturmian basis is somewhat superior for all Z, except that for capture into individual excited states and into all states, the 120-Sturmian basis is superior since these channels are omitted from the 281-Sturmian basis.

Qualitatively, for all targets, the cross sections at their peak energies, and especially at higher energies, obey the same scaling rules as in the appropriate perturbative limits: multiplying the capture cross sections by Z^7 and the excitation and ionization cross sections by Z^4, and scaling the energy by dividing by Z^2, yields curves tending toward universal curves as the energy is increased. At scaled energies near a cross section's peak, most individual scaled cross sections appear to approach a high-Z limit as Z is increased, though not always monotonically, with the greatest change in each case being from $Z = 2$ to $Z = 3$. The change with increasing Z at a scaled cross section's peak is monotonic for capture into the ground state and all states, as previously roughly observed, and also for capture or excitation into individual states (except for $2s$ excitation from He^+ being out of order), but not for excitation to all states or for ionization. Except for $Z = 2$, the spread of scaled cross sections at their peak is narrow: For example, the scaled peak $2p$ direct excitation cross section is $1.6 \times 10^{-16}\ \text{cm}^2 \pm 6\%$ at a scaled energy $v^2 \approx 0.8 \pm 0.1$.

[1] T. G. Winter, G. J. Hatton, and N. F. Lane, Phys. Rev. A **22**, 930 (1980).
[2] M. Kimura and W. R. Thorson, Phys. Rev. A **24**, 3019 (1981).
[3] L. F. Errea, J. M. Gómez-Llorente, L. Méndez, and A. Riera, J. Phys. B **20**, 6089 (1987).
[4] G. Hose, Phys. Rev. A **51**, 2222 (1995).
[5] T. G. Winter, Adv. At. Mol. Opt. Phys. **52**, 391 (2005).
[6] J. Macek and S. Alston, Phys. Rev. A **26**, 250 (1982).
[7] 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.
[8] T. G. Winter, Phys. Rev. A **35**, 3799 (1987).
[9] T. G. Winter, Phys. Rev. A **25**, 697 (1982).
[10] T. G. Winter, Phys. Rev. A **33**, 3842 (1986).
[11] C. D. Stodden, H. J. Monkhorst, K. Szalewicz, and T. G. Winter, Phys. Rev. A **41**, 1281 (1990).
[12] T. G. Winter and S. G. Alston, Phys. Rev. A **45**, 1562 (1992).
[13] T. G. Winter and J. R. Winter, Phys. Rev. A **61**, 052709 (2000). This and later papers corrected for the uneven distribution of Sturmian-generated hydrogenic energies at the ionization threshold.
[14] T. G. Winter, Phys. Rev. A **56**, 2903 (1997).
[15] T. G. Winter, Phys. Rev. A **69**, 042711 (2004).
[16] R. Shakeshaft, Phys. Rev. A **14**, 1626 (1976).
[17] Following Shakeshaft [18] and in earlier work, the highest positive energy s state after diagonalizing the target Hamiltonian is neglected to reduce computing time, probably negligibly affecting the reported cross sections.
[18] R. Shakeshaft, Phys. Rev. A **18**, 1930 (1978).
[19] D. R. Bates, Proc. R. Soc. A **247**, 294 (1958).
[20] T. G. Winter, Phys. Rev. A **80**, 032701 (2009).
[21] The "errors"noted here are generally with $R_{\max} = 80$—smaller, for the most part, than with $R_{\max} = 60$.
[22] This difference is averaged over 50, 75, and 150 keV.

[23] These few larger differences from 100-Sturmian results are as follows: $\leqslant$12% for ground-state and total capture from B^{4+} at 200–600 keV; $\leqslant$18% for ground-state and total capture from C^{5+} up to 625 keV; and two units in the last digit for total capture from Be^{3+} at 1000 keV and C^{5+} at 1500 keV, for which the cross sections are very small.

[24] These exceptions are for capture to $2s$ at 200 keV and to $2p$ at 100–150 keV, for which differences are 23% and 30%, respectively.

[25] For the higher-Z targets, there are these differences of up to two units in the last digit: for excitation of Li^{2+}, 4% at 100 keV and 15–16% at 200–400 keV for $3s$, and 6–8% at 125–400 keV for $3p$; for excitation of Be^{3+}, $\leqslant$9% for $3s,3p$ excitation at 150–1000 keV; and for excitation of B^{4+}, $\leqslant$8% for $2s,3s,3p$ at 400 and 1500 keV. There are small additional differences exceeding one unit: $\leqslant$4%, $\leqslant$2% for direct excitation of the $2s,2p$ states at some energies $\geqslant$200 keV.

[26] T. G. Winter and C. D. Lin, Phys. Rev. A **29**, 567 (1984).

[27] T. G. Winter and C. D. Lin, Phys. Rev. A **29**, 3071 (1984); **30**, 3323(E) (1984).

[28] T. G. Winter, Phys. Rev. A **37**, 4656 (1988).

[29] B. H. Bransden, C. J. Noble, and J. Chandler, J. Phys. B **16**, 4191 (1983).

[30] B. Peart, K. Rinn, and K. Dolder, J. Phys. B **16**, 1461 (1983).

[31] M. F. Watts, K. F. Dunn, and H. B. Gilbody, J. Phys. B **19**, L355 (1986).

[32] J. F. Reading, A. L. Ford, and R. L. Becker, J. Phys. B **15**, 625 (1982).

[33] Xiao-Min Tong, D. Kato, T. Watanabe, and S. Ohtani, J. Phys. B **33**, 5585 (2000).

[34] A. L. Ford, J. F. Reading, and R. L. Becker, J. Phys. B **15**, 3257 (1982).

[35] H. C. Brinkman and H. A. Kramers, Proc. Acad. Sci. Amsterdam **33**, 973 (1930).

[36] The ionization peaks were not observed for all Z by the author in the previously noted work [8] with smaller bases, since the energy ranges were somewhat more limited; except for $Z = 2$, the range of cross sections at the peak for ionization with the smaller basis would appear to be about $\pm$8%. Direct excitation was not considered at all.