# **Electron transfer and ionization in collisions between**  $H^+$ **,**  $He^{2+}$ **,**  $Li^{3+}$ **,**  $Be^{4+}$ **,**  $B^{5+}$ **,**  $C^{6+}$ **,**  $N^{7+}$  **ions** and target  $C^{5+}(1s)$  ions studied using a Sturmian basis

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Cross sections have been determined for electron transfer and ionization in collisions between  $H^+$ ,  $He^{2+}$ , Li<sup>3+</sup>, Be<sup>4+</sup>, B<sup>5+</sup>, C<sup>6+</sup>, N<sup>7+</sup> ions and target C<sup>5+</sup>(1s) ions for projectile energies 125–1000 keV/amu using a coupled-Sturmian-pseudostate approach [Phys. Rev. A 35, 3799 (1987)]. A comparison is made with results using simpler approaches, and rules for scaling with the projectile nuclear charge are considered. Except for  $H^+$ , the results for electron transfer to the ground state are estimated to be converged to 1%; for ionization, the convergence is probably to  $10-20 %$ . [S1050-2947(97)08610-1]

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### **I. INTRODUCTION**

Electron transfer and ionization in collisions between the bare ions  $H^+$ , He<sup>2+</sup>, Li<sup>3+</sup>,... and a specific hydrogenic target ion such as  $C^{5+}(1s)$  is a basic class of atomic collision processes. A decade ago, the author considered collisions between protons and the hydrogenic ions  $He^+(1s)$ ,  $Li^{2+}(1s),...,C^{5+}(1s)$  [1]; see also Refs. [2–6] for more recent work. Studies of the two sets of processes together address the dependence on both projectile and target nuclear charges, and the two have in common the  $H^+$ - $C^{5+}(1s)$  collisional system. The present study was initially motivated by the need for reliable  $\text{He}^{2+}$ -C<sup>5+</sup>(1*s*) electron-transfer cross sections to explain anomalously high  $\alpha$ -particle losses in the tokamak fusion test reactor  $(TFTR)$  [7]. The only available quantal calculation, using a Coulomb-projected Born approximation, gave cross sections orders of magnitude too small  $[8]$ , and it was not obvious whether the results for proton projectiles by the author [1] could be scaled to  $\alpha$ particles at the required intermediate energies.

As in the previous study  $[1]$ , the present one employs a coupled-Sturmian-pseudostate approach  $[9-11]$ . The twocenter Sturmian basis, if extended to completeness, yields exact cross sections not only for transfer but also for ionization. In practice, of course, the need to truncate any basis limits the accuracy. Following a brief summary of the method in Sec. II A, greater detail will be given in Sec. II B on the numerical accuracy and in Sec. III A on the extent of basis convergence. The relationship of cross sections to those obtained with simpler approximations and possible scaling rules will be described in Secs. III B and III C for electron transfer and ionization, respectively. Atomic units are used unless otherwise indicated.

#### **II. METHOD**

### **A. Basic approach**

The coupled-Sturmian-pseudostate approach has been described in detail  $[11]$  and will only be summarized briefly here for the one-electron systems being considered. A bare projectile of charge  $Z_A$  is incident on a hydrogenic ion of nuclear charge  $Z_B$ . At the intermediate projectile energies of interest (and, indeed, at somewhat lower energies), the nuclear motion may be assumed to be classical and at constant velocity. The problem then reduces to solving the timedependent Schrödinger equation for the electron in the timevarying nuclear potential at each impact parameter  $\rho$ . The electronic wave function is expanded here in terms of a twocenter basis of approximate atomic wave functions, some with positive eigenvalues, representing ionization. The square of an expansion coefficient is asymptotically the probability of transition to a particular atomic state of direct excitation, electron transfer, or ionization. The approximate atomic wave functions are obtained by diagonalizing the separated atomic Hamiltonians using Sturmian functions. ~Other basis functions can also be used; see, for example, Refs.  $[5, 6, 12]$ .) The Sturmians are simply radial polynomials multiplied by spherical harmonics and *fixed* exponentials  $e^{-Zr/(l+1)}$ , where *Z* is the nuclear charge, *l* is the orbital angular momentum, and *r* is the electronic radial coordinate appropriate to each nuclear center. Since the exponential is fixed for each *l* and since the polynomials form a complete set, so do the Sturmians.

### **B. Numerical accuracy**

# *1. Sensitivity to choices of numerical parameters*

As in previous work using a coupled-Sturmian approach [1,11], there are four parameters on which the *numerical* accuracy of probability times impact parameter  $\rho P(\rho)$  depends. The cross section *Q* is obtained by integrating  $\rho P(\rho)$ over  $\rho$ . Tests of sensitivity to each of these parameters have been performed for all projectile charges  $Z_A = 2 - 7$  and  $Z_B$  $=6$  at the smallest and largest projectile energies,  $E=125$ and 1000 keV/amu, for a small and a large contributing value of  $\rho$ , 0.125 and 0.75. Tests consisted of the following.

 $(1)$  The lower and upper truncation-error limits in integrating the coupled equations over  $z = vt$  using Hamming's method [13]—change from the production values  $5\times10^{-6}$ ,  $5\times10^{-4}$  to the test values  $5\times10^{-7}$ ,  $5\times10^{-5}$ .

 $(2)$  The range of *z* in integrating the coupled equations change from the production range  $-100$ ,  $+100$  to the test  $range -200, +200.$ 

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TABLE I. Cross sections (in units of  $10^{-19}$  cm<sup>2</sup>) for electron transfer to the ground state in collisions between bare ions of charge  $Z_A$  and target  $C^{5+}(1s)$  ions vs projectile energy *E*.

					$E$ (keV/amu)				
$Z_A$	Approximation	125	250	375	500	625	750	875	1000
1	<b>OBK</b>	0.0201	0.0955	0.165	0.199	0.202	0.188	0.165	0.142
	2-state	0.0186	0.0187	0.0557	0.0865	0.0985	0.0968	0.0883	0.0772
	55-Sturmian	0.0323	0.117	0.133	0.140	0.154	0.132	0.0892	0.0585
	60-Sturmian	0.0321	0.112	0.158	0.135	0.119	0.114	0.109	0.0826
$\overline{2}$	<b>OBK</b>	1.12	4.35	6.60	7.26	6.93	6.15	5.25	4.38
	2-state	0.426	1.02	2.25	2.80	2.79	2.53	2.18	1.84
	55-Sturmian	0.748	3.18	4.17	4.06	3.49	2.79	2.14	1.62
3	<b>OBK</b>	21.5	56.4	68.0	64.7	56.0	46.4	37.8	30.5
	2-state	3.48	11.5	18.2	18.9	17.0	14.3	11.8	9.64
	55-Sturmian	5.42	21.8	26.9	24.9	20.6	16.3	12.6	9.76
4	<b>OBK</b>	305	424	373	297	229	176	136	106
	$2$ -state	26.8	63.0	72.3	64.1	52.5	41.9	33.3	26.5
	55-Sturmian	33.5	81.6	87.4	75.7	61.0	47.8	37.2	28.8
5	<b>OBK</b>	2840	1800	1160	788	555	404	301	229
	2-state	158	185	166	132	102	78.9	61.5	48.4
	55-Sturmian	171	195	174	142	112	87.7	68.5	53.7
6	<b>OBK</b>	7590	3220	1830	1180	809	583	434	331
	2-state	323	254	213	169	131	102	80.3	63.9
	55-Sturmian	334 <sup>a</sup>	256	212	172	138	110	87.9	70.5
7	<b>OBK</b>	3040	2040	1380	979	721	546	423	334
	2-state	132	147	148	133	113	93.2	76.8	63.5
	55-Sturmian	136	157	153	138	119	100	83.8	69.9

<sup>a</sup>45-Sturmian value.

~3! The range beyond which the charge-exchange matrix elements are neglected—change from the production value 30 to the test value 40.

 $(4)$  The number of integration points in the double numerical integration over the spheroidal coordinates  $(\lambda,\mu)$  to calculate the charge-exchange matrix elements—change from the production values of 16  $\lambda$  and 24  $\mu$  points at 125 keV/amu (24  $\lambda$  and 32  $\mu$  points at 1000 keV/amu) to the test values of 24 and 32 points at  $125 \text{ keV/amu}$  (32 and 80 points at  $1000 \text{ keV/amu}$ .

In almost all cases, the tests have been carried out with the 55-state basis usually used in the productions runs  $[14]$ . For parameter 3, the sensitivity is in all cases less than 0.01%. For the other three parameters, the sensitivity is at most 0.1% for transfer (whether to the ground state or to all states) and usually  $\lfloor 15 \rfloor$  for ionization as well. The sensitivity does not appear to depend systematically on  $Z_A$ . However, for the case  $Z_A = 1$ ,  $Z_B = 6$  studied previously [1], the *percent* sensitivity for some parameters is greater (up to  $1-2\%$ ), in part owing to the smallness of the values of  $\rho P(\rho)$ .

# *2. Sensitivity to the number of points needed to calculate the integrated cross section Q*

Simpson's rule has been used in integrating over impact parameter  $\rho$  to obtain the cross section  $Q=2\pi\int \rho P(\rho)d\rho$ using 14  $\rho$  points over the interval 0–1.25, larger  $\rho$  contributing negligibly. As a test of the accuracy of this  $\rho$  mesh, cross sections have been recalculated for all  $Z_A$  and projectile energies *E* using only ten points. Differences are usually less than  $1\%$ , but are up to  $2\%$  for transfer (whether to the ground state or to all states) and 6% for ionization at the smaller energies  $E \le 375$  keV/amu, for which  $\rho P(\rho)$  peaks at smaller values of  $\rho$ . For these cases, cross sections have been recalculated using 18 points (a halved mesh for  $\rho$  $\leq$  0.25). Differences between 14- and 18-point values are at most 0.1% for transfer and 0.4% for ionization. This is estimated to be the accuracy with respect to Simpson's rule integration for all the cross sections for  $Z_A = 2 - 7$  reported here using 14 points. The accuracy for  $Z_A = 1$  using 8–15 points was previously noted to be at least about  $0.5\%$  [1].

#### **III. RESULTS**

Multistate cross sections for electron transfer to the ground state in collisions between the projectile nuclei  $p, \alpha$ ,  $Li^{3+}$ , Be<sup>4+</sup>, B<sup>5+</sup>, C<sup>6+</sup>, N<sup>7+</sup> and the target ion C<sup>5+</sup>(1*s*) are given in Table I for projectile energies from 125 to 1000  $keV$ /amu relative to the target. (The results for protons expand the energy range reported previously  $[1]$ .) (Also shown for later comparison are two-state and first-order results.) Cross sections for electron transfer to all available states are given in Table II. The results for  $Z_A = 2$  are about a factor of three smaller than values obtained using Olson's classical  $code [7]$ ; neither theoretical cross section is sufficiently large to explain anomalous  $\alpha$ -particle losses in the TFTR [7]. The overall excited-state electron-transfer cross section can be obtained by subtracting the multistate results in Table I from those in Table II. Cross sections for ionization are given in Table III.

			$E$ (keV/amu)						
$Z_A$	Approximation	125	250	375	500	625	750	875	1000
1	55-Sturmian	0.0469	0.136	0.178	0.171	0.181	0.155	0.116	0.0772
	60-Sturmian	0.0440	0.142	0.192	0.167	0.147	0.138	0.133	0.108
2	55-Sturmian	0.808	3.60	4.86	4.68	3.93	3.18	2.55	1.98
	classical		14.2		15.3	13.2	10.7		
3	55-Sturmian	5.65	23.6	29.7	27.8	23.4	18.9	15.0	11.7
$\overline{4}$	55-Sturmian	34.3	85.3	93.2	83.1	68.7	55.1	43.6	34.4
5	55-Sturmian	175	202	184	155	127	102	82.0	65.6
6	55-Sturmian	344 <sup>a</sup>	270	232	196	164	137	113	93.6
7	55-Sturmian	154	182	193	185	169	150	130	112

TABLE II. Cross sections (in units of  $10^{-19}$  cm<sup>2</sup>) for electron transfer to all states in collisions between bare ions of charge  $Z_A$  and target  $C^{5+}(1s)$  ions vs projectile energy *E*.

<sup>a</sup>45-Sturmian value.

Cross sections for electron transfer to all states and for ionization are also graphed in Fig. 1. It is seen that, with the exception of the resonant case  $\left[ C^{6+} - C^{5+}(1s) \right]$ , the electrontransfer cross sections all peak in the calculated energy range. All cross sections vary smoothly and simply over several orders of magnitude. There is a regular progression from  $Z_A \ll Z_B$ , where ionization dominates transfer, to  $Z_A \approx Z_B$ , where the reverse is true. The variation with projectile charge  $Z_A$  is more pronounced for electron transfer than for ionization. (Interestingly, ionization cross sections for  $Z_A = 2 - 7$  lie within a quite narrow band at intermediate energies.) More detailed scaling rules and the relationship to simpler approximations will be discussed in Secs. III B and III C.

### **A. Basis convergence**

Results are reported here using 55 states: the Sturmians up to  $9s_A$ ,  $6p_{0,1A}$ ,  $5d_{0,1A}$ ,  $9s_B$ ,  $9p_{0,1B}$ ,  $5d_{0,1B}$  (with the very-high-lying hydrogenic state 9s<sub>B</sub> removed after diagonalizing the  $C^{5+}$  Hamiltonian), one of the larger bases used in the author's previous work  $[1]$ , in which the target rather than projectile nuclear charge was varied. As a test of basis convergence, results have also been determined here using only 45 states at the lowest and highest projectile energies for each projectile charge  $Z_A = 2 - 7$ . A comparison is shown in Table IV  $[16]$ . In the 45-state basis, the highest *s*, *p*, and *d* states on each center have been removed. It is seen that for transfer to the ground state, differences are very small: at most 0.9%. In spite of the greater difficulty of representing excited states, basis differences for transfer into all states are also small: at most 0.6% at the lowest energy and 2.7% at the highest energy; indeed, the basis sensitivity of the excitedstate transfer cross section (obtained by subtraction) is small [17]. For ionization, differences are larger: 8–23%. Barring any basis instability, it seems likely that results with a larger basis, say a 65-state basis, would differ by smaller amounts from the 55-state results than the differences between the 55 and 45-state results. Sufficiently small cross sections, however, have limited basis stability. This is the case for the previously reported results for  $Z_A = 1$  (proton projectiles) [1]: 55- and 60-state transfer cross sections differ by 10–20%, and cross sections now calculated at additional energies show some spurious structure, probably reflecting incomplete basis convergence; see Fig. 1 and Tables I and II.

# **B. Comparison with simpler results for ground-state electron transfer**

#### *1. Relation between two-state and multistate cross sections*

As can be seen in Fig. 2, for almost all studied projectiles incident on  $C^{5+}(1s)$  targets at almost all studied energies,

TABLE III. Cross sections (in units of  $10^{-19}$  cm<sup>2</sup>) for ionization in collisions between bare ions of charge  $Z_A$  and target  $C^{5+}(1s)$  ions vs projectile energy *E*.

		$E$ (keV/amu)							
$Z_A$	Approximation	125	250	375	500	625	750	875	1000
1	55-Sturmian	0.113	0.668	1.30	1.77	2.02	2.14	2.17	2.13
	60-Sturmian	0.120	0.694	1.26	1.72	2.02	2.14	2.19	2.16
2	55-Sturmian	0.162	1.72	3.92	5.61	6.79	7.35	7.44	7.35
3	55-Sturmian	0.157	2.00	5.34	8.74	11.7	13.7	14.9	15.6
4	55-Sturmian	0.193	2.12	5.61	9.56	13.5	17.0	19.7	22.1
5	55-Sturmian	0.328	2.27	5.49	9.24	13.5	18.2	22.8	26.6
6	55-Sturmian	0.411 <sup>a</sup>	2.32	5.33	8.88	13.5	19.0	24.5	29.6
7	55-Sturmian	0.456	2.04	4.75	8.26	13.0	19.1	26.4	32.2

<sup>a</sup>45-Sturmian value.



FIG. 1. Multistate (55-Sturmian) cross sections for electron transfer to all states (circles and solid curves) and ionization (crosses and dashed curves) in collisions between fully stripped ions of charges  $Z_A = 1 - 7$  and  $C^{5+}(1s)$  ions.

the two-state cross section in Bates's approach  $\lceil 18,19 \rceil$  is *less* than the multistate  $(\geq 55$ -state) cross section, which is itself exact in the large-basis limit  $[20]$ . Averaged over energy, the two-state cross section is 35% less than the multistate cross section for  $Z_A = 1$ , the difference decreasing monotonically to only 4% for the symmetric case  $(Z_A=6)$ , and increasing slightly to 6% by  $Z_A = 7$ . This decrease to  $Z_A = 6$  also holds at individual energies for lower intermediate energies *E*  $\leq 625$  keV/amu [21].

Averaged over  $Z_A$ , the difference is greatest (34%) at the tabulated energy  $E = 250 \text{ keV/amu}$ , and decreases monotonically to only 2% at 1000 keV/amu; that the difference is greatest at  $E = 250 \text{ keV/amu}$  and subsequently declines also



FIG. 2. Difference of two-state from multistate (55-Sturmian) cross sections for electron transfer to the ground state in collisions between fully stripped ions of charges  $Z_A = 1 - 7$  and  $C^{5+}(1s)$  ions.  $~(For Z<sub>A</sub>=1,$  the multistate cross section used here is the average of the 55- and 60-state values.)

holds for individual  $Z_A = 1 - 4$ , as can be seen in Fig. 2. For  $Z_A \ge 5$ , the difference is somewhat greater at the highest energy. For all  $Z_A$ , at sufficiently large  $E$ , the two-state approximation of course breaks down, since ionization channels make an important contribution to the transfer cross section there  $[22]$ . At 1000 keV/amu, however, the two-state cross section is as yet too low by only  $8-10\%$  for  $Z_A$  $=4 - 7.$ 

# *2. Relationship between first-order OBK and two-state cross sections*

The first-order Oppenheimer-Brinkman-Kramers (OBK) [23] cross section is the high-energy limit of the two-state cross section in Bates's approach  $[18,19]$ . At the intermediate energies  $E = 125 - 1000$  keV/amu considered here, however, it is generally a poor approximation to the two-state cross section: Averaged over energy, the first-order cross section is 2.4–9.6 times greater than the two-state cross section, and the ratio increases monotonically with  $Z_A$  for  $Z_A$ 

TABLE IV. Differences of 45- from 55-state cross sections for electron transfer to the ground state, all states, and for ionization in collisions between bare ions of charge  $Z_A$  and target  $C^{5+}(1s)$  ions at the projectile energies  $E=125$  and 1000 keV/amu.

		Transfer to the ground state		Transfer to all states	<b>Ionization</b>		
$Z_A$	$125 \text{ keV}^{\text{a}}$	$1000 \text{ keV}^{\text{a}}$	$125 \text{ keV}$	$1000 \text{ keV}$	$125 \text{ keV}^{\text{a}}$	$1.000 \text{ keV}$	
2	$-0.009\%$	$-0.9\%$	$-0.04%$	$-2.7\%$	$-15%$	$-9%$	
3	$-0.5%$	$-0.4%$	$-0.5%$	$-0.7\%$	$-11\%$	$-10%$	
$\overline{4}$	$-0.7\%$	$-0.8%$	$-0.6%$	$-0.1\%$	$-15%$	$-9%$	
	$-0.2%$	$-0.4%$	$-0.1\%$	0.2%	$-22%$	$-13%$	
6	$-0.09\%$	$0.04\%$	0.01%	$-0.3%$	$-23%$	$-14%$	
	$-0.06%$	$-0.2%$	0.02%	$-1.7%$	$-8%$	$-9%$	

<sup>a</sup>250 keV/amu for  $Z_A = 6$ .



FIG. 3. Ratio of first-order OBK to two-state cross sections for electron transfer to the ground state in collisions between fully stripped ions of charges  $Z_A = 1 - 7$  and  $C^{5+}(1s)$  ions.

 $=1-7$ . As can be inferred from Fig. 3, this monotonic increase holds also for each  $E \ge 400$  keV/amu and, for the most part, at lower energies as well.

Averaged over  $Z_A$ , the ratio decreases monotonically from 12.3 to 3.8 as *E* increases from 125 to 1000 keV/amu. As shown in Fig. 3, this monotonic decrease also holds for individual  $Z_A \ge 3$ ; for  $Z_A = 1 - 2$ , the ratio has a maximum value  $(4.3-5.1)$  at the tabulated energy 250 keV/amu and then decreases monotonically at higher energies.

Note in summary that for smaller  $Z_A$  the first-order cross section is sometimes closer to the multistate cross section than to the two-state cross section. This is fortuitous: it is due to successive improvements (first-order→two-state  $\rightarrow$ multistate) generally being of opposite sign.

#### *3. Peak in the electron transfer cross section*

*a. Energy dependence.* The projectile energy at which the first-order (OBK) cross section peaks has been determined here in closed form as a function of  $Z_A$  for transfer to the ground state. The peak energy decreases monotonically as  $Z_A \rightarrow Z_B$  from above or below. If  $Z_A \ll Z_B$ , then the scaled peak energy (in units of 25 keV/amu) is  $E/(25Z_B^2)$  $=(v/Z_B)^2 \approx 2/3$  [1,3,24]. If  $Z_A \approx Z_B$ , then the peak occurs at  $v^2 \approx 4(Z_A - Z_B)^2$ . Specifically, for  $Z_B = 6$ , the scaled peak energy decreases from 0.64 at  $Z_A = 1$  to 0.56 at  $Z_A = 2$  to 0.09 at  $Z_A = 5$ .

The multistate approach qualitatively follows this trend for transfer to the ground state (as well as transfer to all states), except for the questionably converged curve for  $Z_A$  $=$  1. However, the dependence on  $Z_A$  is less dramatic: the scaled peak energy  $(v/Z_B)^2$  decreases from 0.47 to 0.28 as  $Z_A$  increases from 2 to 5; and for  $Z_A = 7$ , the multistate peak is at 0.32, compared to only 0.10 at the OBK peak. The value of  $(v/Z_B)^2$  at the peak for the two-state curve is, not surprisingly, close to that for the multistate curve for  $Z_A=4, 5,$  and 7, differing by at most  $0.04$  (13%), reflecting the similarity of the two-state and multistate curves for  $Z_A$  not very different from  $Z_B$ , as noted in Sec. III B 1. For the symmetric case  $(Z_A = Z_B = 6)$ , the coupled-state curves peak at presumably finite but lower energies than those being considered here  $[E \ge 125 \text{ keV/amu}, (v/Z_B)^2 \ge 0.14]$ ; it is of only academic interest that the OBK cross section peaks at zero energy for this case, since, as noted in Sec. III B 2, it is generally a poor approximation to the coupled-state cross section even at intermediate energies.

*b. Magnitude.* The *magnitude* of the peak in the firstorder  $(OBK)$  cross section  $Q$  can also be determined in closed form. If  $Z_A \ll Z_B$ , then  $Q(Z_A)/Q(1) \cong Z_A^5$  at fixed scaled energy  $(v/Z_B)^2$  [1,3]. For  $Z_A = 1 - 7$  and  $Z_B = 6$  considered here,  $Z_A$  is not much less than  $Z_B$  (nor, in view of this and as shown in Sec. III B 3 a, does the peak energy scale with  $Z_B^2$ ). Nevertheless, the magnitude of the peak is still roughly proportional to  $Z_A^5$ :  $Q(Z_A)_{peak}/Q(1)_{peak} = Z_A^n$ , where *n* increases from 5.15 to 5.97 as  $Z_A$  increases from 2 to 5, and is 4.97 at  $Z_A = 7$ .

For the multistate cross section, *n* decreases from 4.8 to 4.4 as  $Z_A$  increases from 2 to 5, and is 3.6 at  $Z_A = 7$ . (The value of *n* for transfer into all states differs from that for transfer to the ground state at each  $Z_A$  by at most 0.1.) In summary, the first-order and exact curves enjoy only approximate power-law scaling with projectile charge.

### **C. Comparison with simpler results for ionization**

## *1. Relation between first-order and multistate cross sections*

Unlike for electron transfer, the first-order (Born) ionization cross section is exact in the high-energy limit  $[25]$ . At all energies, the multistate cross section is exact if sufficiently converged. For the finite  $(55-60\text{-state})$  basis used here, the multistate ionization cross section is not nearly as accurate as the multistate transfer cross section for  $Z_A$  $=$  2 $-7$ , but has at least been estimated to be converged to 10–20%.

*a. Energy dependence.* The *energy dependence* of the first-order ionization cross section scales simply as  $Z_B^2$  and is independent of  $Z_A$  [25]. The scaled energy (in units of 25  $keV/amu$ ) at the peak in the cross section is approximately  $(v/Z_B)^2 = 1.1$  [i.e., energy  $E = 1000$  keV/amu for the C<sup>5+</sup> target considered here]. In contrast, the peak energy of the multistate cross section varies significantly with  $Z_A$  and, except for the smaller values of  $Z_A$ , exceeds the highest energy  $(E=1000 \text{ keV/amu})$  given in Table III. Results of additional multistate calculations show that the scaled peak energy varies from  $(v/Z_B)^2$ =0.96–0.99 [26] for  $Z_A$ =1, 0.97 for  $Z_A$ = 2, to 2.69 for  $Z_A$ = 7. At least for  $Z_A$ = 2 to 7, the increase is monotonic and, indeed, closely linear for  $Z_A \ge 4$ .

*b. Magnitude.* The magnitude of the first-order ionization cross section scales simply as  $Z_A^2$  at all energies [25]. This scaling is only approximate for the multistate cross section, varying with  $Z_A^n$ , where *n* decreases monotonically from 1.8–1.9 at  $Z_A = 2$  or 3 to 1.6–1.7 at  $Z_A = 7$ . In both energy dependence and magnitude, it is not surprising that the multistate cross section follows the first-order scaling more closely for the more asymmetric systems, for which transitions are less likely and perturbation theory is more applicable.

## **CONCLUSION**

Using a coupled-state approach with a two-center Sturmian basis, cross sections have been determined for electron transfer and ionization in intermediate-energy collisions between bare ions of charges  $Z_A = 1 - 7$  and the specific hydrogenic ion  $C^{5+}(1s)$ . This complements an earlier study in which the target nuclear charge was instead varied. For  $Z_A$  $=2-7$ , cross sections are estimated to be converged to 1%

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- [16] The 45- and 55-state bases exclude *d* states with  $m=2$ . To test the effect of excluding these states, additional, 49-state calculations were made, in which the states  $3d_{2A}$ ,  $4d_{2A}$ ,  $3d_{2B}$ , and  $4d_{2B}$  were included. These tests were carried out for  $Z_A = 2, 4$ , and 6;  $E = 125$  and 1000 keV/amu; and  $\rho = 0.125$  and 0.5. For

for transfer to the ground state, 3% for transfer to all states, and 10–20% for ionization. The cross sections vary smoothly with projectile charge, and roughly obey the scaling rules of first-order perturbation theory.

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electron transfer to the ground state, differences between 45 and 49-state values of  $\rho P(\rho)$  are at most 0.2% (0.4% for transfer to all states); for ionization, differences are at most 2% except for some very small values of  $\rho P(\rho)$ .

- [17] For  $Z_A = 2$  and  $E = 1000$  keV/amu, the excited-state components with the 55- and 45-state bases are, respectively, 18.2% and 16.6%, a ''difference'' of 1.6%; other differences are at most 1%.
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