Electron transfer and ionization in collisions between protons and the ions Li^{2+} and He^{+} studied with the use of a Sturmian basis

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Total cross sections are reported for electron transfer in collisions between protons and Li^{2+} ions at proton energies 17.5—200 keV relative to the Li^{2+} ion and for ionization at energies 50—200 keV. A coupled-state, Sturmian approach has been taken. For electron transfer, a detailed, basis-convergence study has been carried out. Larger-basis results have also been obtained for electron transfer in p-He^{+} collisions, confirming the accuracy of results reported previously with smaller bases, and p-He^{+} ionization cross sections are also reported for the first time with a Sturmian basis. For the p-Li^{2+} processes, results are compared with the only previously existing pseudostate results (one-and-a-half-center results), and, for electron transfer, the energy range of existing results is extended. There do not appear to be any experimental results for p-Li^{2+} collisions. A detailed comparison with the other theoretical results and with experimental results is carried out for the p-He^{+} processes; except for some discrepancies at the extrema of the energy range, the results are in general accord.

I. INTRODUCTION

Electron transfer in collisions between the fully stripped ions He^{2+}, Li^{3+}, ... and hydrogen atoms is of fundamental importance. These processes are the simplest examples of electron transfer in asymmetric systems which are accidentally resonant for some excited final states. They have been studied in detail both theoretically and experimentally, at least for not-too-asymmetric systems.[1] Cross sections at keV energies are reasonably large, and hence comparatively easy to calculate or measure.

Perhaps equally important is the class of "inverse processes": electron transfer in collisions between protons and the hydrogenic ions He^{+}, Li^{2+}, ..., initially in the ground state. These processes are the simplest examples of electron transfer in asymmetric systems which are nonresonant for *all* final states. Since the cross sections are much smaller than those for the first class of asymmetric processes, they are substantially harder to obtain either theoretically or experimentally. With the exception of the first process in the second class, for which the target is the ion He^{+}, very little work has been done on this class of processes.

The basic theoretical difficulty in treating these processes is that the electron does not always proceed directly to the proton, but, rather, often passes through a series of continuum intermediate states which bridge the large energy gap between the tightly bound initial state and the more loosely bound final state. This continuum must be accounted for. Further, the coupling among the bound atomic states cannot be ignored at keV energies. The potentially most fruitful approaches are the coupled-pseudostate approaches. In these approaches, a partial basis of bound atomic states is augmented by pseudostates in one of several forms. When the Hamiltonian of the initial hydrogenic ion or the final hydrogen atom is diagonalized in this augmented basis, some of the eigenvalues are found to be positive, thereby discretely representing the continuum. Therefore, a by-product of any pseudostate calculation is a potentially reliable ionization cross section. Ionization in collisions between protons and hydrogenic ions is also of basic importance.

For the first example—collisions between protons and He^{+} ions—both electron transfer *and* ionization cross sections have been calculated using various pseudostate bases: two-center, pseudostate bases with inclusion of united-atom orbitals;[2,3] two-center, 23-state Callaway-Wooten pseudostate bases;[4] and one- and one-and-a-half-center pseudostate bases.[5] In addition, detailed cross sections only for electron transfer have been reported by this author using two-center, Sturmian pseudostate bases.[6] At the time these results were reported, it was felt that the Sturmian bases were too small and the eigenvalues too sparsely distributed to yield ionization cross sections. New, larger-basis results will show that these smaller Sturmian bases in fact yield surprisingly stable cross sections for ionization.

For collisions between protons and He^{+} ions, several sets of experimental results exist for electron transfer,[7–9] and two sets of results, for ionization.[7,8]

Not nearly as many pseudostate results have been published for the next example—collisions between protons and Li^{2+} ions; only the one- and one-and-a-half-center pseudostate calculations have been carried out for this collision[10] as well as the preceding one, with both electron transfer and ionization cross sections having been reported. There do not appear to be any experimental data for this process.

Since the p-He^{+} and p-Li^{2+} collisions are closely related, the present study using a Sturmian basis is a natural outgrowth of the preceding one. The primary intent here is to provide accurate cross sections for electron transfer in p-Li^{2+} collisions[11] at energies both below and above the cross section's peak. At the lower energies, this will provide a previously unknown cross section. At the same

time, the range of validity of the one-and-a-half-center calculation for this process will be estimated; the one-and-a-half-center method may be unreliable at lower energies, where ionization is less probable than electron transfer, although it appears to serve quite well at higher energies.

Ionization cross sections of substantial accuracy will also be reported as a by-product of this calculation. In addition, new larger-basis cross sections will be reported for electron transfer in p-He^+ collisions, which will establish the accuracy of Winter's previous results.[6] At the same time, previously unreported Sturmian cross sections will be presented for ionization in p-He^+ collisions. By combining the Sturmian and (where available) other results for electron transfer and ionization in p-He^+ and p-Li^{2+} collisions, one can begin to obtain an overview of collisions between protons and hydrogenic ions.

II. METHOD AND NUMERICAL TESTS

The Sturmian approach was first applied to electron transfer in p-H collisions by Gallaher and Wilets[12] and was carried significantly further by Shakeshaft,[13] who also estimated ionization cross sections for the first time with this basis. Winter extended the Sturmian approach to electron transfer in any collision between a bare nucleus and a hydrogenic ion; the extension was detailed, but straightforward. The coupled equations and the equations for the matrix elements are given in Winter's paper and will not be repeated here. Only a summary of the basis functions will be given.

For each angular momentum l, the radial parts of the Sturmian basis functions are simply polynomials multiplied by a fixed exponential $\exp[-Zr/(l+1)]$ (where Z is the nuclear charge and r is the electron-nuclear distance in atomic units). As the number and order of the polynomials centered on each nucleus is increased, the basis inherently approaches completeness, since the polynomials themselves do.

In the remainder of this section, numerical tests and limits of accuracy will be described, since these may differ from those in the previous paper.

The coupled equations have again been integrated using Hammings' method started by a Runge-Kutta integration; here, however, the absolute truncation error has been kept between 5×10^{-6} and 5×10^{-4} rather than 1×10^{-6} and 1×10^{-4} as in that paper. The use of these less stringent error limits significantly reduces the computing time required, while probability is still conserved in almost all cases to within 1×10^{-5}. [For smaller impact parameters ρ or for cases where the capture probability $P(\rho)$ is larger, probability is sometimes conserved to only 1×10^{-4}.] Comparing peak values of $\rho P(\rho)$ using both sets of limits indicated that the less stringent limits still ensure accuracy to at least 0.1% at all energies.

The total cross section Q is again obtained by numerical integration (usually by means of Simpson's rule):

$$Q=2\pi\int_0^\infty \rho P(\rho)$$

(in units of a_0^2), where $P(\rho)$ denotes any probability of interest. A sufficient number of integration points ρ is used (6 or 12–15 points) to ensure that those integrated cross sections reported to three digits are accurate to at least about 0.5%, and those reported to two digits are accurate to about 1–3%.

The charge exchange matrix elements have again been evaluated by double numerical integration over the spheroidal coordinates λ and μ using the procedure described in the previous paper. As a test, peak values of $\rho P(\rho)$ for electron transfer into all states were repeatedly calculated using different numbers of integration points. Based on this test, the numbers of integration points in λ and μ for the larger-bases calculations were increased from 8 and 12 (or 16) to 24 and 32, respectively, as the proton's energy was increased from 17.5 to 200 keV; this ensures that values of $P(\rho)$ are generally stable to 0.1% and that probability is conserved to the extent noted in the previous paragraph. (The only exception is for p-Li^{2+} collisions at 17.5 keV, where only 8 λ and 12 μ points were used; here the estimated accuracy is 0.35%.) In the previous paper, the numbers of integration points at larger energies were smaller, due to the greater ease of integrating with a smaller basis.

Finally, the integration of the coupled equations was carried out over the interval $z=vt$ from $-100a_0$ to $+100a_0$, with the charge exchange matrix elements zeroed for $|z|>40a_0$. Tests for p-Li^{2+} collisions with larger ranges indicate that these cutoffs do not cause errors in the capture probabilities greater than 0.02%; the same ranges were previously used for p-He^+ collisions.

III. RESULTS

The Sturmian cross sections for electron transfer and ionization in collisions between protons and the ions He^+ and Li^{2+} are graphed in Fig. 1 and listed in Tables I and II. Also shown in Fig. 1 for later comparison in Sec. III B are the only other coupled-pseudostate results for all four processes: the one-and-a-half-center results of Reading, Ford, and Becker[5] and Ford, Reading, and Becker.[10] Other pseudostate results for p-He^+ electron transfer and ionization will also be compared in that section, and experimental results for these processes will be compared in Sec. III C.

On the basis of detailed convergence tests to be described in Sec. III A, the Sturmian results for electron transfer are estimated to be reliable to at least 2–10% and 5–15% for p-He^+ and p-Li^{2+} collisions, respectively, over the entire energy ranges considered, with the greater accuracy at the lower energies. For p-He^+ electron transfer, these results are scarcely changed from the smaller-basis values previously reported by Winter.[6] Detailed convergence studies have not been carried out for ionization; the ionization cross sections, however, are probably reliable to 10–20%, perhaps more.

Thus, the cross sections displayed in Fig. 1 may be considered to be reasonably accurate representations of the true cross sections. What follows in this paragraph is a summary of their chief features. All of the cross sections are "small," the largest—the p-He^+ electron transfer cross section—not exceeding 0.3 $Å^2$. For p-Li^{2+} collisions, both the capture and ionization cross sections are about an order of magnitude below the corresponding

TABLE I. Coupled-Sturmian cross sections (in units of Å^2) for electron transfer and ionization in collisions between protons and He^+ ions vs proton energy E relative to the $^4He^+$ ion. The collision energy with respect to the center-of-mass reference frame is $0.8E$.

E (keV)	Number of basis functions[a]	Electron transfer 1s	Electron transfer all[b]	Ionization
17.5	19[c]	0.0917	0.0979	
17.5	35	0.0911	0.0964	
31.25	24[c]	0.213	0.233	
50	24	0.235	0.268	0.0379
50	35[d]	0.230	0.272	0.0399
75	24	0.172	0.207	0.0743
150	24	0.0452	0.0611	0.108
150	35	0.0443	0.0583	0.108

[a]The 19—24-state Sturmian results for electron transfer were reported previously by Winter in Ref. 6.
[b]Cross sections marked "all" are for electron transfer into all *available* bound states.
[c]The 19 functions $1sA$, $2sA$, $3sA$, $2p_{0,1}A$, $1sB, \ldots, 5sB$, $2p_{0,1}B, \ldots, 4p_{0,1}B$, $3d_{0,1,2}B$, where A and B refer to the proton and He nucleus, respectively, and the 24 functions $1s\alpha, \ldots, 6s\alpha$, $2p_{0,1}\alpha$, $\alpha = A, B$, $3p_{0,1}B, \ldots, 6p_{0,1}B$.
[d]The above 24 functions $+7s\alpha$, $\alpha = A, B$, $3p_{0,1}A$, $7p_{0,1}B$, $8p_{0,1}B$, $3d_{0,1,2}B$.

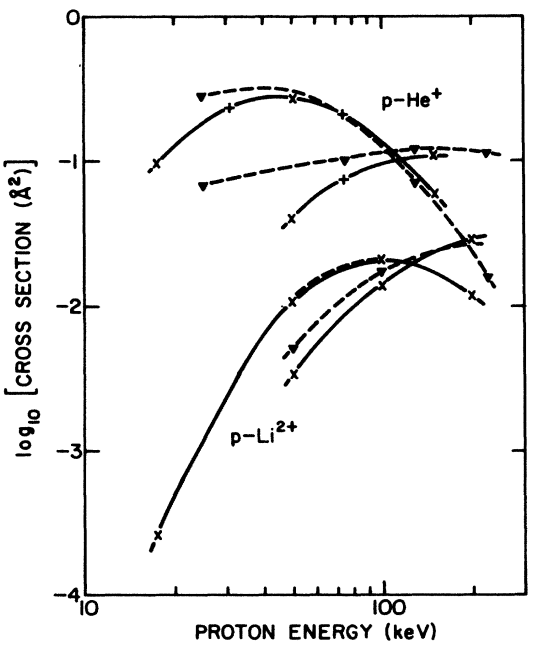

FIG. 1. Theoretical cross sections for electron transfer into all states of H and for ionization in collisions between protons and the ions He^+ and Li^{2+}. The upper and lower four curves are for He^+ and Li^{2+}, respectively. In each group of four curves, the pair of curves declining more rapidly at the higher energies is for the electron transfer, while the other pair is for ionization. Crosses and plus signs: two-center, Sturmian pseudostate using, respectively, 35—38 and 19—26 functions (respectively, this work and previous work, Ref. 6); triangles: one-and-a-half-center pseudostate (Reading, Ford, and Becker, Ref. 5 for p-He^+ collisions and Ford, Reading, and Becker, Ref. 10 for p-Li^{2+} collisions). The curves are intended only to guide the eye. One-and-a-half-center points coinciding with Sturmian points have been omitted for clarity.

cross sections for p-He^+ collisions. The p-Li^{2+} curves peak at higher energies than do the p-He^+ curves; e.g., the p-Li^{2+} electron transfer curve peaks at a proton energy of 100 keV, twice the energy for the p-He^+ case.[14] Qualitatively, these features are, of course, due to the tighter binding of an electron initially in the $Li^{2+}(1s)$ ion than in the $He^+(1s)$ ion.

It is instructive to consider also graphs of $\rho P(\rho)$ versus ρ, shown in Figs. 2 and 3 for electron transfer and ionization, respectively. It is seen that for electron transfer and ionization in p-Li^{2+} collisions, the $\rho P(\rho)$ curves peak at smaller values of ρ than in p-He^+ collisions, as expected, since the initial $Li^{2+}(1s)$ orbital is more compact than the initial $He^+(1s)$ orbital. In all cases, only a small range $\rho \lesssim 3.5a_0$ is required to obtain accurate integrated cross sections Q. Further, the $\rho P(\rho)$ curves are not very energy dependent; all curves have a single peak, nearly the same at all energies for a given target ion,[15] and the electron transfer curves are only a little broader than the ionization curves, and otherwise of the same shape. This is not inconsistent with the strong dependence of electron transfer on continuum intermediate states except at energies lower than those considered here.

A. Basis convergence studies

As a follow-up to the previously published study by Winter for p-He^+ electron transfer,[6] a detailed Sturmian-basis convergence study has been carried out for p-Li^{2+} electron transfer. In addition, p-He^+ electron transfer cross sections have been recalculated with a much larger basis than those previously used, in order to test directly the convergence estimates previously made.

Potentially reliable ionization cross sections are a by-product of pseudostate calculations of electron transfer cross sections. Previously, it was felt to be premature to report p-He^+ ionization cross sections with the smaller

TABLE II. Coupled-Sturmian cross sections (in units of Å^2) for electron transfer and ionization in collisions between protons and Li^{2+} ions vs proton energy E relative to the $^7Li^{2+}$ ion. The collision energy with respect to the center-of-mass reference frame is $0.875E$.

E (keV)	Number of basis functions	Electron transfer $1s$	Electron transfer all[a]	Ionization
17.5	26[b]	0.000 24	0.000 27	
17.5	38[c]	0.000 230	0.000 269	
50	26	0.0096	0.011	0.0028
50	36[c]	0.008 80	0.0106	0.003 38
100	26	0.019	0.023	0.015
100	36	0.0175	0.0207	0.0139
200	23[b]	0.012	0.014	0.028
200	36	0.009 52	0.0118	0.0285

[a]Cross sections marked "all" are for electron transfer into all *available* bound states.
[b]The 26 functions $=19$ functions (as in Table I, but for Li^{2+})$+4sA$, $5p_{0,1}B$, $6p_{0,1}B$, $4d_{0,1,2}B-5sB$, where nucleus B is the Li nucleus; in the 23-function basis, the functions $4d_{0,1,2}B$ are removed.
[c]The 38 functions $1s\alpha,\ldots,7s\alpha$, $2p_{0,1}\alpha,\ldots,5p_{0,1}\alpha$, $3d_{0,1}\alpha$, $4d_{0,1}\alpha$, $\alpha=A$, B, $+8sB-\overline{8sB}$; the 36 functions $1s\alpha,\ldots,6s\alpha$, $2p_{0,1}\alpha,\ldots,5p_{0,1}\alpha$, $3d_{0,1}\alpha$, $\alpha=A$, B, $7sA-\overline{6sB}+6p_{0,1}B$, $7p_{0,1}B$ at 50 keV. At the two higher energies, the functions $6p_{0,1}A$ are added, and $3d_{0,1}A$, removed. The line over $6sB$ or $8sB$ indicates an approximate hydrogenic state formed by diagonalizing the Li^{2+} Hamiltonian in the Sturmian basis.

Sturmian bases then used, which yielded only very sparse distributions of positive-energy eigenvalues; however, a comparison of results with these bases and the present larger basis reveals an encouraging degree of stability.

1. *Electron transfer*

This is the most direct test of the convergence of any coupled-state calculation: simply to add a large block of functions to an existing basis and note its effect. Referring to Table I, it is seen that substantially enlarging the 19—24 Sturmian bases (by 50% or more) leaves virtually unchanged the p-He^+ electron-transfer cross sections previously reported: the effect is less than 2% at the two lower energies and only 4.6% at the highest energy. (The effect is at most 2% at all energies if only transfer to the ground state is considered.) These small effects are quite consistent with the effects that could be inferred from the previously published convergence studies at selected impact parameters using smaller bases. Since the additional block of states is a large, representative sample of additional states of several angular momenta, it seems unlikely that further additions would have a significant effect.

For electron transfer in p-Li^{2+} collisions, smaller bases of 23—26 functions have been constructed of size and character similar to those of the smaller bases used in treating p-He^+ collisions. These bases have then been enlarged to include 36—38 functions, guided by the detailed convergence study to be described below. (A larger basis of similar size and character was then employed in the p-

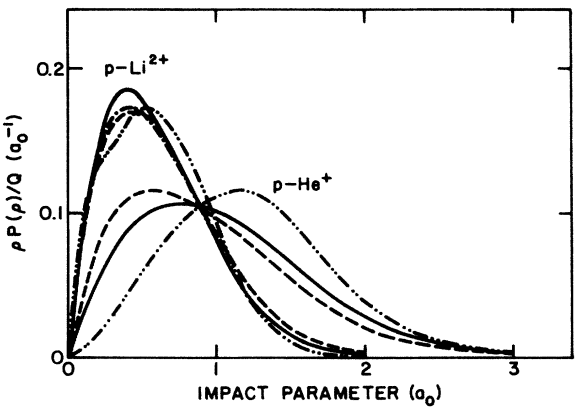

FIG. 2. Normalized probabilities times impact parameter $\rho P(\rho)/Q$ vs impact parameter ρ for electron transfer into all states of H in p-He^+ collisions (lower curves) and p-Li^{2+} collisions (higher curves) at various proton energies E. Solid curves: $E=50$ keV; dashed curves: $E=150$ keV (p-He^+ collisions), 100 keV (p-Li^{2+} collisions); dash-dotted curve: $E=200$ keV; dash-double-dotted curves: $E=17.5$ keV. The area under each curve is $(2\pi)^{-1}$. The bases are the 35—38 Sturmian "production bases" described in the footnotes to Tables I and II.

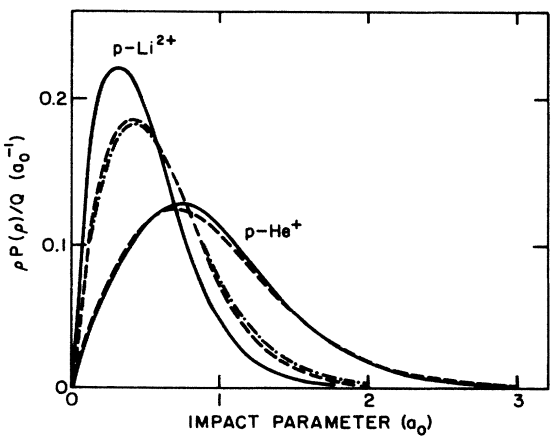

FIG. 3. Normalized probabilities times impact parameter $\rho P(\rho)/Q$ vs impact parameter ρ for ionization in p-He^+ and p-Li^{2+} collisions at various proton energies. The notation is otherwise as in Fig. 2.

He^+ calculations noted above.) By referring to Table II, it is seen that the difference between the smaller- and larger-basis cross sections ranges from 3–5% at the two lower energies to 12–16% at the two higher energies. (These comparisons are for electron transfer into all states; the changes for ground-state electron transfer are up to 5% larger.) It is to be expected that the changes would be larger than for p-He^+ collisions, since the only approximately represented continuum is probably more important for p-Li^{2+} collisions. However, in view of the study which follows, the overall accuracy of the larger-basis results is probably still at least 5–15%.

The $\rho P(\rho)$ curves for p-Li^{2+} electron transfer in Fig. 2 are almost unchanged when the size of the basis is substantially changed: curves (not shown) using the 23–26 functions are very similar to those shown using the 36–38 functions. (These smaller-basis curves for 50- and 100-keV protons are only a little more compact.) All the curves have a single peak at $\rho \simeq 0.5a_0$. Thus, the following study at this single-impact parameter should provide a good estimate of the accuracy of the integrated cross sections.

In Tables III and IV are listed values of $\rho P(\rho)$ for numerous bases of progressively increasing size. Table III indicates the effects of adding Sturmian functions centered on the proton (nucleus A), and Table IV, the effects of adding functions centered on the Li nucleus (nucleus B). [These tables list values of $\rho P(\rho)$ for electron transfer into all states of H; tables for electron transfer into the ground state are omitted for brevity.] It is seen that the first few s and p functions centered on each nucleus have large effects on the order of at least 20% each. The effects then diminish and roughly alternate in sign as the "principal quantum number" n of each function is increased; the oscillations are damped with respect to adding more and more functions of a given angular momentum l and center. The wavelengths of the oscillations appear to increase with l, making it more and more difficult to assess the extent of convergence; however, for $l \geq 1$, the amplitudes of the oscillations do appear to be smaller, the larger the angular momentum. The detailed structure of the oscillations depends on which other basis functions are present; note, for example, the two studies of the effects of s functions centered on nucleus A for 50-keV protons; the presence of some other highly excited states, perhaps centered on another nucleus, may increase the

TABLE III. The role of Sturmian functions centered on the proton (nucleus A): Probability times impact parameter for electron transfer into all states of H in collisions between protons and Li^{2+} ions for various bases. The impact parameter has been fixed at $0.5a_0$. The energy E is the proton's energy relative to the Li^{2+} ion.

Basis functions[a,b]	E (keV)=17.5	17.5	50	50	100	200
17,30 functions[c]			0.005 09		0.0072	0.003 11
$+2sA$			0.007 49	0.005 44	0.0117	0.006 32
$+3sA$			0.008 62	0.006 22	0.0144	0.009 54
$+4sA$	0.000 159		0.008 96	0.006 59	0.0132	0.007 62
$+5sA$	0.000 166		0.008 70	0.006 59	0.0127	0.006 62
$+6sA$	0.000 171		0.008 80	0.007 04	0.0138	0.007 24
$+7sA$	0.000 165	0.000 173	0.008 82	0.006 78	0.0130	0.006 96
$+8sA$	0.000 161	0.000 169	0.008 85	0.006 52	0.0130	0.007 04
$+9sA$	0.000 161		0.008 86	0.006 40	0.0129	0.006 98
$+10sA$	0.000 162		0.008 81	0.006 39[f]	0.0129	0.006 91
20,25 functions[d]						
$+3p_{0,1}A$	0.000 189					
$+4p_{0,1}A$	0.000 213	0.000 225				
$+5p_{0,1}A$	0.000 222	0.000 240	0.008 93		0.0112	0.006 83
$+6p_{0,1}A$	0.000 228		0.009 18		0.0122	0.007 32
$+7p_{0,1}A$					0.0119	0.007 14
20 functions			0.008 96		0.0132	0.007 62
$+3d_{0,1,2}A$	0.000 164		0.009 27		0.0134	0.007 66
$+4d_{0,1,2}A$	0.000 172		0.009 38		0.0136	0.007 71
$+5d_{0,1,2}A$	0.000 170		0.009 20		0.0135	0.007 65
33 functions[e]	0.000 229					
$+4f_{0,1,2,3}A$	0.000 228					

[a]In a given row, the basis in each group consists of all functions listed down to and including those in that row.

[b]The following bases are referred to below and in Table IV: the 24-function basis $1s\alpha, \ldots, 4s\alpha, 2p_{0,1}\alpha, \ldots, 4p_{0,1}\alpha$, $\alpha = A, B, 5sB, 3d_{0,1,2}B$ and the 29-function basis $=24$ functions $-3d_2B + 3d_{0,1}A, 4d_{0,1}\alpha$, $\alpha = A, B$.

[c]The 17 functions $=24$ functions (in footnote b) $-2sA, \ldots, 4sA, 3p_{0,1}A, 4p_{0,1}A$ except for the right columns at 17.5 and 50 keV; the 30 functions $=29$ functions $-2sA, \ldots, 4sA + 5p_{0,1}\alpha$, $\alpha = A, B$, at 17.5 keV (right column); and the 30 functions $=24$ functions $-2sA, \ldots, 4sA, 3d_{2B} + 5p_{0,1}A, 3d_{0,1}A, 6sB - \overline{6sB} + 5p_{0,1}B, \ldots, 7p_{0,1}B$ at 50 keV (right column).

[d]The 20 functions $=24$ functions $-3p_{0,1}A, 4p_{0,1}A$ except at 17.5 keV (right column), for which the basis is 25 functions $=29$ functions $-3p_{0,1}A, 4p_{0,1}A$.

[e]The 29 functions $+3d_2\alpha, 4d_2\alpha$, $\alpha = A, B$.

[f]The functions $3d_{0,1}A$ are omitted (the effect of this omission being estimated to be less than 0.2%).

TABLE IV. The role of Sturmian functions centered on the Li nucleus (nucleus B): Probability times impact parameter for various bases. The parameters and notation are as in Table III except where noted.

Basis functions	E (keV)=17.5	17.5	50	100	200	200
18 functions[a]	0.000 415[f]					
$+4sB$	0.000 218[f]					
$+5sB$	0.000 159[f]		0.008 96	0.0132	0.007 62	
$+6sB$	0.000 170[f]		0.007 87	0.0137	0.007 27	
$+7sB$	0.000 162[f]		0.007 74	0.0136	0.007 30	
$+8sB$	0.000 159[f]		0.008 02	0.0133	0.007 33	
21,22 functions[b]	0.000 159		0.007 87	0.0137	0.007 27	
$-\overline{8sB}$	0.000 159					
$-\overline{7sB}$	0.000 169					
$-\overline{6sB}$	0.000 170		0.007 74	0.0135	0.007 20	
14,25 functions[c]			0.011 01	0.0210	0.012 36	
$+2p_{0,1}B$			0.006 54	0.0148	0.010 89	
$+3p_{0,1}B$	0.000 173		0.007 27	0.0109	0.008 63	
$+4p_{0,1}B$	0.000 159	0.000240	0.008 96	0.0132	0.007 62	
$+5p_{0,1}B$	0.000 164	0.000190	0.007 81	0.0146	0.008 88	
$+6p_{0,1}B$	0.000 165	0.000192	0.007 73	0.0133	0.009 02	
$+7p_{0,1}B$	0.000 164	0.000190	0.008 21	0.0127	0.008 82	
$+8p_{0,1}B$	0.000 167		0.008 01	0.0128	0.008 62	
17,25 functions[d]	0.000 151[f]				0.007 67	0.007 60
$+3d_{0,1,2}B$	0.000 159[f]		0.008 96	0.0132	0.007 62	0.007 57[g]
$+4d_{0,1,2}B$	0.000 168[f]		0.008 85	0.0131	0.007 49	0.007 44[g]
$+5d_{0,1,2}B$	0.000 164[f]		0.008 87	0.0130	0.007 29	0.007 29[g]
$+6d_{0,1,2}B$					0.007 06	0.007 07[g]
29 functions[e]	0.000 225		0.009 09	0.0132	0.007 44	
$+4f_{0,1}B$	0.000 229		0.009 09	0.0132	0.007 44	

[a]The 24 functions (in footnote b, Table III) $-3p_{0,1}A$, $4p_{0,1}A$, $4sB$, $5sB$.
[b]The 21 functions =24 functions $-3p_{0,1}A$, $4p_{0,1}A+6sB$; the 22 functions =21 functions (just noted) $-4sA+7sB$, $8sB$.
[c]The 14 functions =24 functions $-3p_{0,1}\alpha$, $4p_{0,1}\alpha$, $\alpha=A$, B, $2p_{0,1}B$ except for a basis of 25 functions =29 functions $+5p_{0,1}A-2p_{0,1}B, \ldots, 4p_{0,1}B$ at 17.5 keV (right column).
[d]The 17 functions =24 functions $-3p_{0,1}A$, $4p_{0,1}A$, $3d_{0,1,2}B$ except for a basis of 25 functions = 29 functions $-3d_{0,1}B$, $4d_{0,1}B$ at 200 keV (right column).
[e]The functions noted in footnote b, Table III.
[f]The function $4sA$ is omitted.
[g]The functions nd_2B are omitted.

role of the excited states being tested. However, viewed over several oscillations, the effects in the two studies are somewhat similar. The convergence question is a multidimensional one. Ideally, the starting basis for a given series of functions being studied (e.g., s functions centered on A) should be converged except with respect to the particular kind of function being tested, but this is not always practical.

A cutoff has been arbitrarily placed on each series: no function tested beyond the cutoff contributes more than 4% to the "converged limit" of $\rho P(\rho)$, i.e., the value obtained with the production basis. This 4% criterion yields cutoffs of $n=6$–8 for s states centered on either nucleus and $n=5$–7 for p states. The bases are not as asymmetric as one might have expected for an asymmetric collision: excited states centered on nucleus A as well as B are required. This may be as much due to the additional variational freedom afforded by functions corresponding to a nuclear charge of one (which happen to be centered on the proton) as to the presence of a specific second functional center. For s states centered on nucleus B (the Li nucleus), the approximate hydrogenic state of largest positive eigenvalue (obtained by diagonalizing the Li^{2+} Hamiltonian in the Sturmian basis) has also been deleted; this state contributes at most 2% to $\rho P(\rho)$, and its presence substantially increases the computing time. Based on the cutoff criterion, d functions at most up to $n=4$ were included, and those centered on A were omitted entirely at the two higher energies. The tested f states were found to contribute at most 2%, as were $m=2$ d states; these states were also omitted. The final bases used in the production runs contain 36–38 functions, and are defined in footnote c of Table II. In all, about 30 functions *beyond* these 36–38 functions were individually tested. Their effects can perhaps best be summarized by noting that the *algebraic* sum of the percent changes due to all these neglected functions tested does not exceed 4% except at the highest proton energy of 200 keV, where the sum is 11%, of which 7% is due to the neglected functions $4d_{0,1}B$, $5d_{0,1}B$, and $6d_{0,1}B$.

2. *Ionization*

Cross sections for ionization in collisions between protons and the ions He^+ and Li^{2+} are listed in Tables I and

II, respectively. Results are shown for the same smaller and larger bases as were used to calculate the electron transfer cross sections. It is seen that for p-He^+ collisions, the smaller-basis ionization cross sections agree very closely (within 1—4%) with the larger-basis values at both proton energies (50 and 150 keV) for which values are given. For p-Li^{2+} collisions, differences at the two lower energies (50 and 100 keV) are somewhat larger (11—17%) than those noted for p-He^+ collisions, while at the highest energy (200 keV), the difference is again very small (1%). This sensitivity to basis size is thus not large even for p-Li^{2+} collisions over the energy range 50—200 keV, and is comparable to that previously indicated for electron transfer in Sec. III A 1. Now, however, the smaller sensitivity is at the *higher* proton energies. This makes sense because ionization is dominant there and because the spectrum of Sturmian-generated eigenvalues, shown in Tables V and VI, contains positive eigenvalues which are generally large (particularly for Li^{2+}) and perhaps more suited to higher-energy collisions, in which there is a greater percentage of higher-energy ejected electrons than in lower-energy collisions. Considering how few eigenvalues there are at the critical low energies which contribute most to the integrated ionization cross section, it is surprising that the smaller bases, in particular, generate reasonable cross sections for ionization at all. Indeed, only at the lowest energy, 17.5 keV (for which ionization cross sections are not shown in Tables I and II), are cross sections for ionization not necessarily converged; positive eigenvalues are probably needed that are smaller than those of even the larger basis. Mukoyama, Lin, and Fritsch[16] have recently reproduced quite well the exact p-H ionization probability density for 25-keV protons (within a semiclassical approximation) for the first two partial waves using a basis of pseudostates for each partial wave which provided only six positive eigenvalues, ranging from 0.05 to 22 a.u., as well as one or two eigenvalues just below the ionization threshold; the cross section obtained by integrating the probability density over electron energies is also correct. The present Sturmian results indicate that even fewer eigenvalues in the low-energy region are required, at least for generating the integrated cross section at not-too-low energies.

B. Comparison with other coupled-state results

1. p-He^+ electron transfer

The two-center, bound-atomic-state (eight-state) results of Bransden and Noble,[17] and of Winter[6] (not shown) are much too low at all proton energies except for 150 keV. (The two sets of bound-state results do agree with each other.) At 150 keV (the highest energy considered here), the surprisingly good agreement (within a few percent) between these results and the Sturmian results, not only in cross section, but also in probability times impact parameter, may be fortuitous. (Capture into all states, it may be noted, is underestimated at this energy by at least 10% using the bound-state basis.) The fact that there are large differences between the Sturmian and bound-state results at most energies in the presently considered range does point to the need to account for the atomic continuum for the p-He^+ electron transfer process.

The atomic continuum is needed not only to represent intermediate ionization states but also, at lower energies, molecular coupling as well. At the lowest energy considered here, 17.5 keV, the 10-molecular-state, plane-wave-factor cross section of Winter, Hatton, and Lane[18] is much closer to the Sturmian result than is the bound-atomic-state result. However, due to the neglect of ionization channels, even this molecular-state result is too low here (by about 25%), although it is acceptable at lower energies, where ionization is unimportant.

Besides the Sturmian results, there are two other sets of two-center results which at least partly account for the continuum by means of pseudostates: the 16-state, augmented-atomic-orbital (AO +) results of Fritsch and Lin;[2] and the 23-state, Callaway-Wooten pseudostate results of Bransden, Noble, and Chandler.[4] The AO + basis includes united-atom orbitals and, in so doing, also partly accounts for ionization channels, as does the other basis. The AO + cross sections agree outstandingly well (within 5%) with the Sturmian results except at the higher energy (150 keV), where the AO + result is about 15% higher; see Fig. 4. (This is a comparison of ground-state cross sections.) This suggests that, at this energy, the comparatively small AO + basis may need to be enlarged, al-

TABLE V. Eigenvalues (in atomic units) of the H and Li^{2+} Hamiltonians using 26 Sturmians. This is the smaller basis employed for p-Li^{2+} collisions. (The $\overline{4dB}$ states have been omitted at 200 keV; see also Table II for a definition of the basis.)

H state[a]	Approximate eigenvalue	Exact eigenvalue	Li^{2+} state	Approximate eigenvalue	Exact eigenvalue
$\overline{1sA}$	−0.5	−0.5	$\overline{1sB}$	−4.5	−4.5
$\overline{2sA}$	−0.1136	−0.125	$\overline{2sB}$	−1.0223	−1.125
$\overline{3sA}$	0.2140		$\overline{3sB}$	1.9261	
$\overline{4sA}$	2.3996		$\overline{4sB}$	21.5962	
$\overline{2p_{0,1}A}$	−0.125	−0.125	$\overline{2p_{0,1}B}$	−1.125	−1.125
			$\overline{3p_{0,1}B}$	−0.4992	−0.5
			$\overline{4p_{0,1}B}$	−0.1829	−0.281 25
			$\overline{5p_{0,1}B}$	0.6231	
			$\overline{6p_{0,1}B}$	4.5590	
			$\overline{3d_{0,1,2}B}$	−0.5	−0.5
			$\overline{4d_{0,1,2}B}$	−0.2143	−0.281 25

[a]The overline indicates an approximate hydrogenic state formed by the basis.

TABLE VI. Eigenvalues of the H and Li^{2+} Hamiltonians using 36 Sturmians. This is the larger basis employed for p-Li^{2+} collisions at proton energies 100–200 keV.

H state	Approximate eigenvalue	Exact eigenvalue	Li^{2+} state[a]	Approximate eigenvalue	Exact eigenvalue
$\overline{1sA}$	−0.5	−0.5	$\overline{1sB}$	−4.5	−4.5
$\overline{2sA}$	−0.1249	−0.125	$\overline{2sB}$	−1.1190	−1.125
$\overline{3sA}$	−0.0324	−0.0555...	$\overline{3sB}$	−0.0684	−0.5
$\overline{4sA}$	0.1257		$\overline{4sB}$	2.3141	
$\overline{5sA}$	0.5127		$\overline{5sB}$	9.9711	
$\overline{6sA}$	1.7087				
$\overline{7sA}$	8.8101				
$\overline{2p_{0,1}A}$	−0.125	−0.125	$\overline{2p_{0,1}B}$	−1.125	−1.125
$\overline{3p_{0,1}A}$	−0.0555	−0.0555...	$\overline{3p_{0,1}B}$	−0.4999	−0.5
$\overline{4p_{0,1}A}$	−0.0203	−0.031 25	$\overline{4p_{0,1}B}$	−0.2458	−0.281 25
$\overline{5p_{0,1}A}$	0.0692		$\overline{5p_{0,1}B}$	0.1691	
$\overline{6p_{0,1}A}$	0.5066		$\overline{6p_{0,1}B}$	1.3905	
			$\overline{7p_{0,1}B}$	7.0611	
			$\overline{3d_{0,1,2}B}$	−0.5	−0.5

[a]The state $\overline{6sB}$ corresponding to the large eigenvalue 56.4023 has been removed.

though it appears quite satisfactory at lower energies. Bransden *et al.* report two sets of pseudostate results: (a) those for pseudostates centered only on the proton, as well as $n \leq 2$ bound atomic states centered on the He nucleus; and (b) those for pseudostates centered only on the He nucleus, as well as $n \leq 2$ bound atomic states centered on the proton. (They note that they would have combined the bases A and B except for some problems of numerical instability.) Graphically interpolating their results of approximation A graphed in Figs. 4 and 5, there is seen to be agreement with the Sturmian results to perhaps 10% at all proton energies of at least 31 keV. The results of their approximation B are lower than those of approximation A by 10–25%. According to Bransden *et al.*, the results of approximation A are expected to be more reliable except at proton energies greater than about 125 keV. The Sturmian results favor the results of approximation A at all energies, including the single energy greater than 125 keV reported here (150 keV).

Consider finally the one-and-a-half-center results of Reading, Ford, and Becker[5] using a very large basis of 54 pseudostates with, however, only one state centered on the proton; this single charge-transferring state is only approximately taken into account. These one-and-a-half-center results are nearly identical (within 9%) with their one-center (target-center) results. At the single proton energy of 75 keV which is approximately the same in both the one-and-a-half-center and the Sturmian results, there is excellent agreement (within 5%). (See Fig. 4.) If, for ground-state electron transfer, one graphically interpolated the Sturmian result at 25 keV and the one-and-a-half-center result at 150 keV, then the one-and-a-half-center results would perhaps be 35% higher and 10% lower, respectively, than the Sturmian values at these energies. The comparison between results for electron transfer into all bound states is less clear, since their use of an n^{-3} rule corresponds to an energy-independent contribution of 20% from excited states, whereas the Sturmian-estimated contribution varies from 6% at the lowest energy to 32% at the highest energy; the results of Bransden *et al.* also reveal an energy-dependent effect from capture into $n=2$ levels alone, varying from about 8% at 26 keV to more than 20% at 228 keV.

The one-and-a-half-center method has so far been applied only using a single projectile-centered state (the ground state), treated perturbatively, augmenting a large target-centered basis. The inclusion of additional pertur-

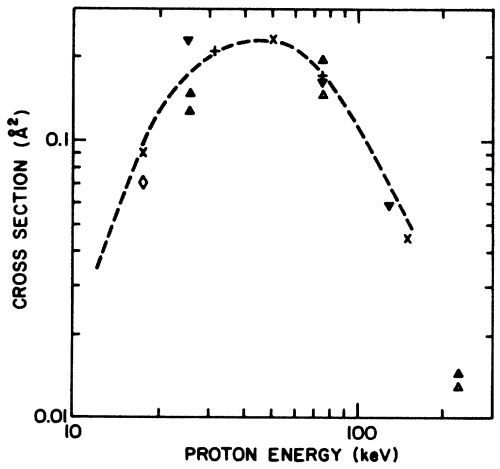

FIG. 4. Coupled-state cross sections for electron transfer into the ground state of H in collisions between protons and He^+ ions at various proton energies relative to the He^+ ion. Crosses: 35-state Sturmian (present results); plus signs: 19–24-state Sturmian (Winter, Ref. 6); dashed curve: 16-state AO+ (Fritsch and Lin, Ref. 2); solid and open triangles: 23-state Callaway-Wooten, approximations A and B, respectively (Bransden, Noble, and Chandler, Ref. 4); inverted triangles: one-and-a-half-center (Reading, Ford, and Becker, Ref. 5); open diamond: molecular with plane-wave factors (Winter, Hatton, and Lane, Ref. 18). Not shown is a one-and-a-half-center point at 227.5 keV nearly coincident with the open triangle there; some low-energy data have also been omitted.

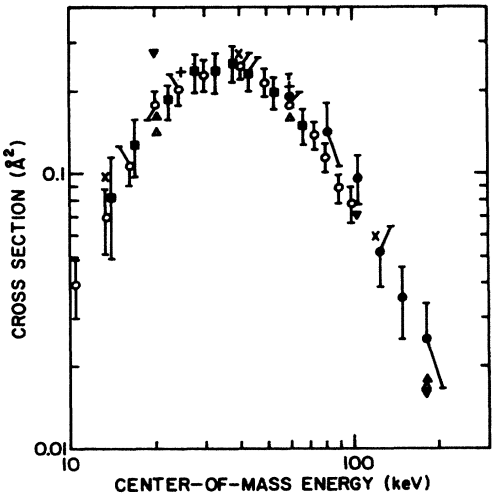

FIG. 5. Coupled-pseudostate and experimental cross sections for electron transfer into all states of H in collisions between protons and $^4He^+$ ions at various collisions energies in the center-of-mass frame. The notation for the theoretical results is as in Fig. 4. The experimental results are as follows. Solid circles: Angel, Sewell, Dunn, and Gilbody (Ref. 7); solid squares: Peart, Rinn, and Dolder (Ref. 8); and open circles: Rinn, Melchert, and Salzborn (Ref. 9). For clarity, the values at about 60 keV of Bransden *et al.* (approximation *A*) and Reading *et al.* have been omitted; these values agree closely with the Sturmian point shown. Also omitted are the AO + values of Fritsch and Lin, given in Fig. 4 for the ground state; when increased to allow for electron transfer into excited states, these values agree closely with the experimental results.

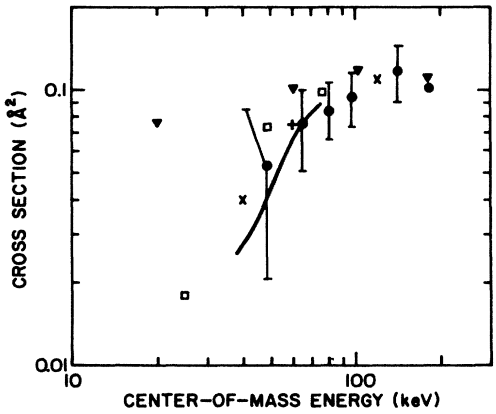

FIG. 6. Coupled-pseudostate and experimental cross sections for ionization in collisions between protons and $^4He^+$ ions as a function of the collision energy in the center-of-mass reference frame. The notation is as in Fig. 5, with the addition that the open squares refer to the 20—23 pseudostate results of Fritsch and Lin (Ref. 3) and the exception that the solid circles with error bars refer to the measurements of Watts, Dunn, and Gilbody (Ref. 7).

batively treated projectile-centered states might be expected to yield better results, and perhaps reduce the estimated 35% difference from the present results at 25 keV, noted above. The inclusion of (nonperturbatively treated) projectile-centered states in the two-center Sturmian pseudostate approach has been noted previously to have a large effect.

In summary, there is very good overall agreement among the coupled-state results over the presently considered energy range 17.5—150 keV. However, neglecting projectile-centered states, or only approximately taking them into account, leads to a significant overestimate of the electron transfer cross section at the lowest energies and perhaps some underestimate at the highest energy. The contribution from excited-state capture is a significant, energy-dependent effect.

2. *p-He⁺ ionization*

Referring to Fig. 6, it is seen that the Sturmian cross sections agree to within at least 20% with the 20—23 pseudostate results of Fritsch and Lin[3] in the overlapping range of energies; there is comparable agreement with the one-and-a-half-center results[10] at center-of-mass energies of at least 70 keV. As the energy is decreased below 70 keV, the one-and-a-half-center results depart more and more from the present Sturmian pseudostate results and the pseudostate results of Fritsch and Lin, probably reflecting the inadequate treatment of electron transfer channels in the one-and-a-half-center calculation when electron transfer dominates ionization.

As is well known, the first Born approximation gives the correct high-energy limit of the ionization cross section. The first Born cross section (not shown) lies above the one-and-a-half-center curve, the difference decreasing from about 20% at 100 keV to about 5% at 200 keV; the one-and-a-half-center and present results appear to be merging at the highest energy, 150 keV, of the present calculation, the difference there being an estimated 12%.

3. *p-Li²⁺ electron transfer*

The only other coupled-pseudostate results available for p-Li^{2+} collisions appear to be the one- and one-and-a-half-center results of Ford, Reading, and Becker;[10] see Fig. 1. [Assuming detailed balancing holds, there also exist coupled-bound-atomic-state results[19] (not shown) for electron transfer into the ground state, but, presumably due to the importance of ionization channels, these results are again substantially below the pseudostate results, as they are for p-He^+ electron transfer.] It is seen that, for electron transfer, the agreement between the Sturmian and one-and-a-half-center results is extraordinarily good: at least 1% at the two higher energies, the difference only increasing to 6% as the proton energy is decreased to 50 keV. (The difference of the Sturmian results from the one-center results increases to 12%.) This comparison is for electron transfer into all states of H, with the n^{-3} rule having been assumed in presenting the one-and-a-half-center results. In a comparison for electron transfer into the ground state, which might be expected to be more definitive, differences are at most 3% at the higher energies, and still only 6% at the lowest energy. Thus, more than for p-He^+ collisions, the approximate treatment of

proton-centered states in the one-and-a-half-center method does not appear to introduce significant error in the electron transfer cross section down to 50 keV (and perhaps somewhat lower energies as well); and the n^{-3} rule appears to be approximately valid over the entire overlapping energy range of the two calculations and, indeed, at least down to 17.5 keV, the lowest energy of the present calculation.

4. p-Li^{2+} ionization

Referring again to Fig. 1, it is seen that for p-Li^{2+} ionization, the relation between the Sturmian and the one-and-a-half-center cross sections is qualitatively similar to that for p-He^+ ionization, the two cross sections in each case rising with energy and appearing to merge roughly with one another at proton energies of about 150 keV. (Contrast this with the case of electron transfer, for which the curves appear to merge at the lower energy of about 50 keV.) For p-Li^{2+} ionization, however, the difference between the two curves is smaller than it is for p-He^+ ionization: at 50 keV, the one-and-a-half-center curve is a factor of 1.5 higher, rather than a factor of 2.3 higher as for the p-He^+ case. In both cases, the differences at the lower energies would be smaller if the Born correction of 10—15% for higher partial waves—perhaps an overestimate at these energies—had been omitted from the one-and-a-half-center calculations.

The first Born cross section[10] (not shown) lies above the one-and-a-half-center curve, the difference decreasing from 14% at 100 keV to 1% at 200 keV, the highest energy considered here; these differences—and generally differences from the present curve as well—are smaller than those noted previously for p-He^+ collisions.

C. Comparison with experimental results

1. p-He^+ electron transfer

The coupled-pseudostate[2,4–6] and experimental results[7–9] for electron transfer into all states of H are shown in Fig. 5. In all cases, the experimental error limits shown are total error limits, i.e., the sums of the estimated random and systematic errors. It is seen that the experimental results are in accord within these limits over the entire energy range. There is excellent general agreement between the coupled-pseudostate and experimental results. Only the lowest-energy, one-and-a-half-center point[5] is significantly above the experimental results; as discussed in Sec. III B, this probably reflects the inadequacy at low energies of the one-and-a-half-center representation of proton-centered states, as well as, to a lesser extent, the overestimate there of capture into excited states using the n^{-3} rule. At the highest energy, the slight discrepancy between this result and the experimental result of Angel, Sewell, Dunn, and Gilbody[7] may reflect an underestimate there of excited-state capture, as previously discussed. The Sturmian results are in complete agreement with the experimental results of Angel *et al.*, available at the higher energies, and of Peart, Rinn, and Dolder,[8] available at the lower energies. The recent data of Rinn, Melchert, and Salzborn[9] spans the lower and part of the higher energy ranges. The Sturmian results also agree with these data, except at the lowest center-of-mass energy, 14 keV, where the Sturmian result is above the upper error limit by 10%. Overall, however, the agreement is excellent.

2. p-He^+ ionization

In Fig. 6 the error limits on the experimental cross sections of Watts, Dunn, and Gilbody[7] are the estimated total error limits. Not shown are the estimated error limits on the measurements of Peart *et al.*[8] and Angel *et al.* (a single point of the latter at the highest energy being shown). Even considering just the displayed error limits on the measurements of Watts *et al.*, the experiments are seen to be in accord. For all the measurements, the experimental procedure of subtraction leads to significant errors at the lower energies, where the cross section for ionization is not large compared to the cross section for electron transfer. In view of this, there is probably agreement, within the range of experimental error, between the Sturmian results (and probably the pseudostate results of Fritsch and Lin[3] as well) and the results of Peart *et al.* as well as those of Watts *et al.* As the energy is decreased, the one-and-a-half-center results differ increasingly from the trend of the experimental results.

Note added in proof. Recently, Professor M. R. C. McDowell and Dr. A. M. Ermolaev have provided the author with cross sections for electron transfer and ionization in p-Li^{2+} collisions. Some of these cross sections are the results of a calculation using a two-center 32-pseudostate basis. For electron transfer into the ground state of H, their results agree with the two-center Sturmian pseudostate results to within 3—9% at the lowest and highest energies of the Sturmian calculations, while differing by about 25% at the intermediate energies 50—100 keV. (Differences of their results for electron transfer from the one-and-a-half-center results of Ref. 10 are similar.) For ionization, their preliminary cross sections are above the Sturmian results by 22—58%. They have also obtained results of a calculation with only one proton-centered state and 27 pseudostates centered on Li^{2+}; these results generally differ from the Sturmian results by somewhat more than do their fully two-center results.

ACKNOWLEDGMENTS

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[15]In fact, over the energy ranges considered, an accurate curve $\rho P(\rho)$ vs ρ for each process at a single energy, together with four points $[\rho,\rho P(\rho)]$ at each energy, sufficed in a sample calculation to reproduce the cross sections to within at least 10% (usually 5%).
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