Coupled-Sturmian and perturbative treatments of electron transfer and ionization in high-energy p-He^+ collisions

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Cross sections have been determined for electron transfer and ionization in collisions between protons and He^+ ions at proton energies from several hundred kilo-electron-volts to 2 MeV. A coupled-Sturmian approach is taken, extending the work of Winter [Phys. Rev. A **35**, 3799 (1987)] and Stodden *et al.* [Phys. Rev. A **41**, 1281 (1990)] to high energies where perturbative approaches are expected to be valid. An explicit connection is made with the first-order Born approximation for ionization and the impulse version of the distorted, strong-potential Born approximation for electron transfer. The capture cross section is shown to be affected by the presence of target basis functions of positive energy near $v^2/2$, corresponding to the Thomas mechanism.

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I. INTRODUCTION

Coupled-pseudostate approaches have proven successful in treating electron transfer and ionization in ion-atom collisions at intermediate energies. There, both processes have significant cross sections. For the simple p-He^+ collision system, these intermediate proton energies range from about 15 keV to a few hundred keV. (The speed of a 25-keV proton equals the orbital speed of a $1s$ electron in hydrogen.) Over this energy range, a coupled-state approach with a basis of about 40 suitably chosen functions yields total electron transfer and ionization cross sections accurate to 10–20%. Such a coupled-state approach has been taken by Winter [1–3] and, recently, by Stodden *et al.* [4] using a Sturmian basis, following earlier work by Shakeshaft [5] and others on the p-H system. Other coupled-state results, as well as experimental results, are cited in Refs. [1–3].

These coupled-state approaches have not heretofore been extended smoothly to high energies in part because it is generally thought that a large number of basis functions would be needed to represent ionization channels, not only to describe ionization, but also its effect on capture: First- and second-order integrated capture cross sections differ significantly—e.g., by about a factor of 2 [6] for the related p-He process at an energy of a few MeV. (Further, the smallness of the capture probability at high energies might make it difficult to extract unless the numerical noise in a coupled-state calculation were kept small.) Reading, Ford, and Becker [7] did include a large number of target-centered functions to represent ionization channels and treated the electron-transfer channel perturbatively in a pioneering "one-and-a-half-center" calculation up to a proton energy of almost 500 keV. However, they did not extend the calculation to MeV energies.

Very recently, Toshima and Eichler [8] reported a high-energy (5-MeV) coupled-state calculation of differential cross sections for electron transfer in symmetric (p-H) collisions and explicitly reproduced the Thomas peak using a fairly large Gaussian basis, but of s functions only. Therefore, they could not simultaneously represent the direct ionization channels, dominated by p waves. On the other hand, a recent coupled-state calculation by Winter [9] using a Sturmian basis considered ionization (and excitation), but not capture, in p-He collisions. The presently considered p-He^+ system is a suitable testing ground for an extension of coupled-state approaches to high energies: It is a prototype asymmetric system, uncomplicated by additional electrons, and it is one for which there are accurate coupled-state results to tie into at lower energies.

Another potential difficulty in extending the coupled-state approaches to high energies is the evaluation of matrix elements. The charge-exchange matrix elements contain a velocity-dependent plane-wave factor which becomes highly oscillatory at MeV energies. Toshima and Eichler used Gaussian orbitals to permit an analytic evaluation of these matrix elements and thereby avoid a high-order numerical integration. However, it will be shown in the present paper that numerical integration with a Laguerre-type (e.g., Sturmian) basis is also feasible.

The outline of the paper is as follows. The method used—the coupled-Sturmian approach for asymmetric, one-electron systems—has been described in Ref. [1] and will not be repeated here. Numerical details differ, however, and these will be presented in Sec. II. The coupled-Sturmian and perturbative results will be described in Sec. III. Atomic units will be used unless otherwise indicated.

II. NUMERICAL TESTS

A. Evaluation of matrix elements

As described in Ref. [1], the velocity-dependent, charge-exchange coupling and overlap matrix elements are evaluated by double numerical integration over the prolate spheroidal coordinates λ and μ. The μ integration from -1 to $+1$ is carried out as before using Gauss-Legendre quadrature and apparently poses no special problem at the higher energies now being considered. A comparison has been made of results obtained using 40- and 80-point quadrature at selected proton energies E and impact parameters ρ. (These tests, and most tests to follow, have been performed with a 35-state basis at $E=450$ keV, $\rho=0.75$ and a 37-state basis at $E=2$ MeV, $\rho=0.25$ and 0.75.) Capture probabilities using 40 and 80 points differ by at most 0.5% and ionization probabilities by at most 0.06%. For all the results reported in this paper, 40-point Gauss-Legendre quadrature has been used.

The integration over the spheroidal coordinate λ is more sensitive. In previous calculations at intermediate energies [1–4], the λ integration from 1 to ∞ was carried out with Gauss-Laguerre quadrature over the transformed coordinate x ranging from 0 to ∞ using up to 32 integration points. (The variable x is defined so that the exponential in the integrand is simply e^{-x}, which is then absorbed into the Laguerre weight.) To test the adequacy of these 32 points at higher energies, additional higher-order zeros and weights, up to 48 points, have been obtained [10]. At $E=450$ keV the 32-point Gauss-Laguerre integration appears adequate: Probabilities for capture and ionization obtained using 32 points differ by at most 0.06% from those using 36 points. The ionization probability is similarly insensitive at 2 MeV, but only because it is little affected there by the capture channel. The capture probability at 2 MeV is itself quite sensitive: 32- and 36-point values differ by 4–38 %, depending on the basis and impact parameter. As the number of points is increased, the differences alternate in sign and appear to dampen. At the dominant impact parameter ($\rho\simeq 0.25$), the difference between 44- and 48-point results is up to a few percent. This accuracy is not entirely satisfactory. Further, some 48-point weights (those corresponding to large zeros x) are very small and do little but cause underflows on some computers.

An alternate, more flexible scheme using Simpson's rule has been adopted. Tests have been carried out at $E=2$ MeV, $\rho=0.25$ with a 35-state basis. The capture probability obtained with an integration over x from 0 to 16 differs by only 0.04% from that obtained with a larger range up to 20; large values $x\sim 100$ appearing in high-order Gauss-Laguerre quadrature are avoided. Keeping $x_{\max}$ fixed at 16, the capture probabilities using 81 and 161 evenly spaced points differ by 3%, and those using 161 and 321 points differ by 0.2%; 161 points are deemed adequate. (The 161-point probability using Simpson's rule differs from the 48-point Gauss-Laguerre value by 1%.) All capture cross sections for $E\geq 700$ keV reported to three digits in this paper, as well as some other results reported to fewer digits, have been calculated using 161 λ points. (The main 2-MeV results may also be numerically reliable to three digits, but in view of the more conservative test to be described in Sec. II C, they are only reported to two digits.)

B. Additional tests

The sensitivity to three other parameters has also been tested. First, the truncation-error limits in integrating the coupled equations, normally between 5×10^{-4} and 5×10^{-6}, have been made 5 times smaller. Tested capture and ionization probabilities at 450 keV and 2 MeV are affected by at most 0.1%. Second, the range beyond which charge-exchange matrix elements are neglected was increased to $50a_0$ from the chosen $40a_0$. The effect on the tested capture and ionization probabilities at 450 keV and 2 MeV is at most 0.04%. Third, the full range over which the coupled equations are integrated was increased from the normal $(-100a_0, 100a_0)$ to $(-200a_0, 200a_0)$; the effect on the capture and ionization probabilities, tested at 2 MeV only, is less than 0.03%. [A range smaller than $(-100a_0, 100a_0)$ would probably also be adequate, since individual excited-state transitions, persisting to large distances, are not being studied here.]

C. Conservation of probability

Conservation of probability provides a conservative overall test of the numerical accuracy both of the evaluation of charge-exchange matrix elements and of the integration of the coupled equations. In the main capture production runs for $E\geq 700$ keV (the results of which will be underlined in the table to be presented later), the summed probability does not differ from unity by more than 10^{-6} at any impact parameter. The error reflected in the capture cross section is estimated to be at most 0.2%, 0.6%, and 10% at 700 keV, 1 MeV, and 2 MeV, respectively. All capture cross sections reported to three digits are estimated to be numerically reliable to better than 1% based on conservation of probability. Conservation of probability also ensures that ionization probabilities, which are larger, are numerically reliable to three digits. The integration over impact parameter to obtain total cross sections is probably accurate to at least 1%.

III. RESULTS

A. Ionization

1. First-order Born approximation

The high-energy limit of the ionization cross section is certainly given by the first-order Born approximation. (The only question is how quickly this limit is reached.) Integrated first-order Born ionization cross sections have been calculated and plotted by Bates and Griffing [11] for collisions between protons and hydrogen atoms. These cross sections can be scaled to collisions between protons and other hydrogenic ions [3] such as He^+, although a comparison with experiment has sometimes called the scaling process itself into question at intermediate energies [12].

In a coupled-state approach, ionization probabilities are calculated one impact parameter at a time and, except for an intractably large basis, are limited to the dominant lower partial waves, those with $l \leq 2$. For the sake of a detailed comparison with coupled-state results, it seems desirable, therefore, to calculate the first-order Born ionization probability a partial wave l and impact parameter ρ at a time. Summed over l and integrated over ρ, the result can be checked explicitly against the scaled cross section of Bates and Griffing. (This also tests the validity of scaling with target nuclear charge, since the present calculation is carried out for He^+ rather than H targets.)

The present nonbasis calculation has been carried out using the formulas for the Coulomb wave function and auxiliary functions in Bethe and Salpeter [13] and Abramowitz and Stegun [14]. Determining the ionization probability for one impact parameter and partial wave entails three numerical integrations (all carried out using Simpson's rule): integrations over the radial electronic coordinate, collision time, and the continuum electron energy.

The present results, summed over partial waves $l \leq 4$, agree to within 3–5 % at 450 keV, 700 keV, 1 MeV, and 3 MeV with the graphical values of Bates and Griffing scaled to He^+ targets. At all energies, the present results are below those of Bates and Griffing, reflecting, at least in part, the small contribution from neglected partial waves. (The graphical uncertainty is perhaps 1–3 %.) As is known, p waves dominate at high energies: The present results show that the p-wave contribution increases slightly from 58% at 450 keV to 64% at 2 MeV. The s- and d-wave contributions decrease from 9% and 21%, respectively, at 450 keV to 7% and 17% at 2 MeV. The f-wave contribution is 5–7 %, and the g-wave contribution is 2–3 %. (These percentages are relative to the scaled values of Bates and Griffing.) The lowest three partial waves thus contain almost 90% of the total-ionization cross section.

2. *Coupled Sturmian*

Consider first the convergence of the ionization probability with respect to the size of the Sturmian basis. Shown in Fig. 1 is the variation of the p-wave probability times impact parameter $\rho P(\rho)$ as the number of target-centered p Sturmians is increased for $E=2$ MeV at $\rho=0.75$, near the peak in $\rho P(\rho)$ vs ρ. It is seen that the probability stabilizes quickly and, indeed, approaches the Born value. As noted previously in the context of the first-order Born approximation, the p-wave contribution dominates the overall ionization probability at high energies. The smaller s and d components also appear to converge and, indeed, converge to the Born values, but more slowly. Each dip in the s-wave component corresponds to the movement of a state to just below the ionization threshold where it is no longer counted as ionization; the sum over ionization channels plus higher-lying bound states appears to converge monotonically. The overall graphs of $\rho P(\rho)$ vs ρ for various partial waves are shown in Fig. 2 at $E=1$ MeV. (Graphs for 700 keV and 2 MeV, not shown, are very similar.) It is seen that for all impact parameters the s and p Sturmian curves agree closely with the corresponding Born curves; indeed, the integrated cross sections for each of these partial waves agree to 3–4 % at all three energies. For the finite partial-wave target basis chosen ($n \leq 12$), the d Sturmian curve at smaller ρ agrees less closely with the Born curve; the integrated d cross section agrees to only 13–14 % at the three energies, reflecting the slower basis convergence previously noted. Summed over the lowest three partial waves, however, the agreement between the Sturmian and Born cross sections is 5–6 %. The neglected higher partial waves, as noted previously, contribute about an additional 10%; see also Fig. 2.

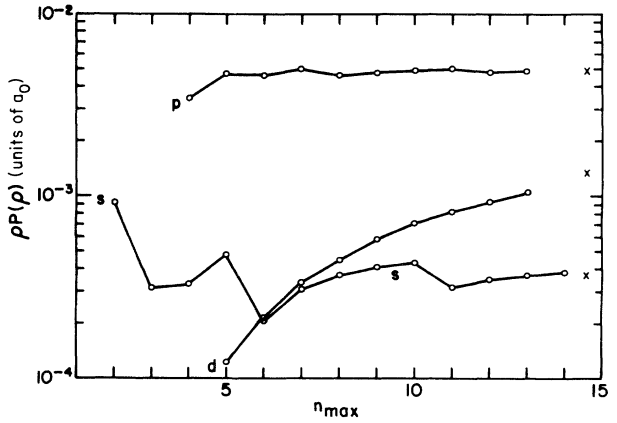

FIG. 1. Probability times impact parameter $\rho P(\rho)$ for ionization in 2-MeV p-He^+ collisions into $l=0,1,2$ partial waves for $\rho=0.75$. Solid curves, coupled-Sturmian including $1s$, $\leq n_{max} lm$ Sturmians centered on the He nucleus (and a $1s$ function centered on the proton, of negligible importance). Crosses, first-order Born approximation (present results).

The bases used in these studies include not only target-(He-) centered states, but also the charge-transfer state $1s$ (centered on the proton). That there is good agreement between the coupled-Sturmian and Born results—within 3–4 % for the more converged partial waves—in part shows that charge transfer plays only a minor role in ionization, at least for the tested energies $E \geq 700$ keV. This was checked explicitly at one impact parameter by calculating ionization probabilities in a large, purely target-centered basis (of 34–36 states) and recalculating them with the $1s_H$ state also included. The effect is at most 0.7% for $E \geq 700$ keV and decreases with increasing energy.

The only slight (3–4 %) disagreement at high energies between the coupled-Sturmian and Born partial-wave cross sections also shows that indirect coupling between target-centered states of a given l—between ionization channels of different energies and between ionization channels and bound excited states—has little effect on ionization. The effect of coupling between states of different l has also been tested by including all states $1s_H$, $\leq 12s,p_{0,1He^+}$ together and comparing the resulting ionization cross section with that obtained with the s and p

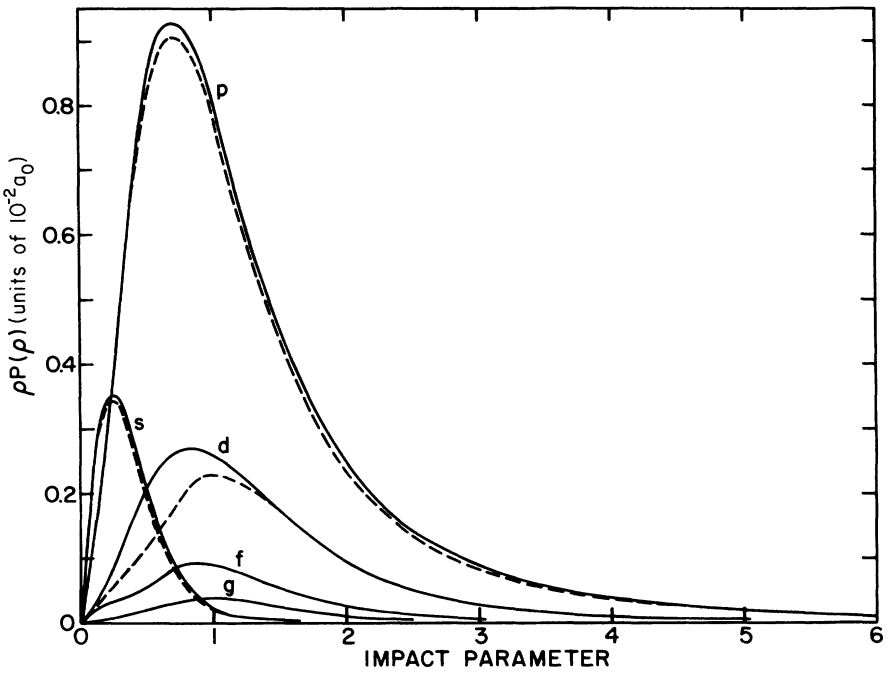

FIG. 2. Probability times impact parameter $\rho P(\rho)$ vs impact parameter ρ for ionization in 1-MeV p-He^+ collisions into $l=0,1,2$ partial waves. Solid curves, first-order Born approximation (present results). Dashed curves, coupled-Sturmian including $1s$, $\leq 12lm$ Sturmians centered on the He nucleus (and a $1s$ function centered on the proton, of negligible importance).

components calculated separately and then combined. The difference is only 1.4% at 700 keV, decreasing to 0.5% by 2 MeV.

These tests for $E \geq 700$ keV show explicitly that ionization is dominated by first-order coupling—i.e., that the first-order Born approximation is valid to a few percent here. This indeed appears true at substantially lower energies as well: As is seen in Fig. 3, the one-and-a-half-center results of Reading, Ford, and Becker [7] obtained with a large target-centered expansion (plus the $1s$ charge-transfer state treated perturbatively [15]) agrees with the Born curve down to 225 keV.

To represent ionization at these energies without a large target-centered basis including d states, a large two-center basis is needed to compensate for this lack: The 35-state basis used previously with success at lower energies [3] is inadequate; containing only $\leq 7s,3p$ states centered on the proton and no d ionization states centered on the He nucleus, it yields a cross section which is irregular beyond 300 keV. (All results for ionization and capture for $E \geq 225$ keV are given in Table I. The best results are plotted in Fig. 3 for these and lower energies.) On the other hand, a basis with still more projectile-centered states—a 51-state basis [4] containing the projectile functions $\leq 8s,8p$, but still lacking d ionization states centered on the He nucleus—does better than the 35-state basis in representing the neglected target partial waves at these transition energies to a purely target-centered process; note the 51-state points at 750 keV in Fig. 3. The projectile-centered expansion has difficulty representing target-centered processes when the translation factor becomes very oscillatory. At high energies the rough completeness of basis functions on one center does little to compensate for the lack of completeness of basis functions on the other.

Theoretical and experimental cross sections for ionization are compared in Fig. 3 for energies of at least about 150 keV. (The theoretical curves are extended to lower energies to show the overall trend. A comparison with experiment was made in Refs. [1–3] for the lower energies. The larger Sturmian basis used in Ref. [4] increases the ionization cross section at these energies by about 30%, but the results still agree with experiment.) Over the energy range 150–500 keV, the first-order Born, one-and-a-half-center, and Sturmian results agree, the slight difference of $\simeq 10\%$ at 300 keV probably reflecting Sturmian basis sensitivity. In the range 150–300 keV, these results all agree with the experimental results of Watts, Dunn, and Gilbody [12]. (All experimental error bars shown are the sum of random and absolute errors.) The three higher-energy experimental points (in the range 300–500 keV) are the total He^{2+} production cross sections of Angel *et al.* [16], from which have been subtracted small capture cross sections. All the theoretical results lie above the upper experimental error bar by about 10% at 380 and 480 keV.

B. Electron transfer

All higher-energy Sturmian cross sections for electron transfer are given in Table I along with the ionization cross sections previously discussed. Those judged best are graphed in Fig. 3, including also lower-energy results to indicate a more complete energy dependence. (The previously determined lower-energy results [1–3] for capture are little affected by enlarging the basis [4], and thus the good agreement with experiment noted in Refs. [1–3] still obtains.) It is seen that there is good agreement between the Sturmian and one-and-a-half-center results [7] in the higher-energy range $\simeq 150-500$ keV (the difference at about 225 keV reflecting different estimates of capture into excited states) and agreement with the experimental results of Watts, Dunn, and Gilbody [12] up to the highest experimental energy, about 225 keV. (The error bars shown are total error limits.) Experimental results at higher energies would be very desirable.

Also shown in Fig. 3 is the impulse version of the distorted strong-potential Born cross section (present results). It has been shown recently that the strong-potential Born approximation [17] within a distorted-wave formalism [18] (DSPB) reduces [19] to the original impulse approximation [20] in the case of pure Coulomb interactions between the particles, as is the situation here. The results presented in Fig. 3 were obtained by using a transverse peaking approximation in the evaluation of the capture amplitude [21]. The DSPB cross section provides the correct limit at high energies (having an error of order $1/v^2$ at finite proton velocities v). The DSPB cross section should have an accuracy at finite velocities comparable to that of the first-order Born approximation of Bates and Griffing for ionization. They are suitable benchmarks against which to compare the present coupled-state results. Indeed, the impulse approximation for capture consists of the ionization amplitude folded with the final, electronic-state momentum distribution. The DSPB approximation, like other second-order approximations for capture, takes account of the two-step (Thomas) mechanism which is very important at high energies; the DSPB approximation has the advantage in the case of asymmetric systems, such as p-He^+, that the quantity Z/v^2 is not assumed small (where Z is the target nuclear charge). It is seen in Fig. 3 that over the entire energy range 30–2000 keV, the multistate Sturmian cross section agrees to within 34% with the DSPB curve. The

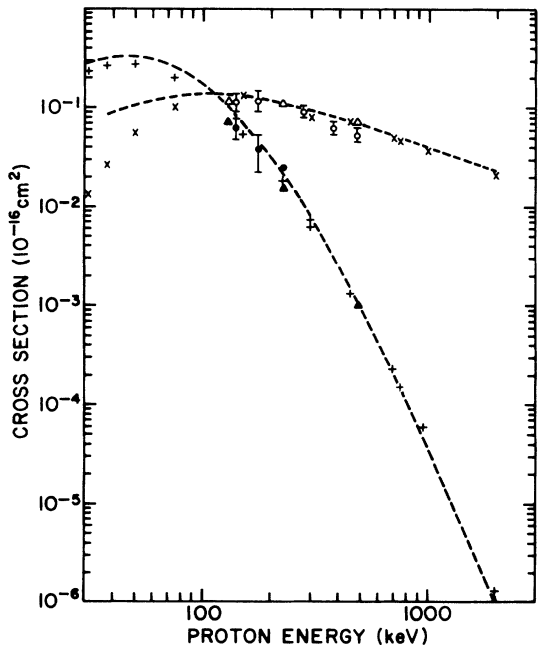

FIG. 3. Cross sections for electron transfer and ionization in p-He^+ collisions. Theoretical results: crosses (ionization) and plus signs (transfer), Sturmian, present results, Winter [3], and Stodden *et al.* [4]; dashed curves, first-order Born, Bates and Griffing [11] for ionization, and distorted strong-potential Born (DSPB), present results for capture; triangles, one-and-a-half-center Reading, Ford, and Becker [7]. Experimental results: circles, Watts, Dunn, and Gilbody [12] and Angel *et al.* [16]. The Sturmian results for ionization at 700 keV, 1 MeV, and 2 MeV include first-order Born contributions from partial waves $l=3,4$; the Sturmian results for capture at these energies include an excited-state fraction of 0.20.

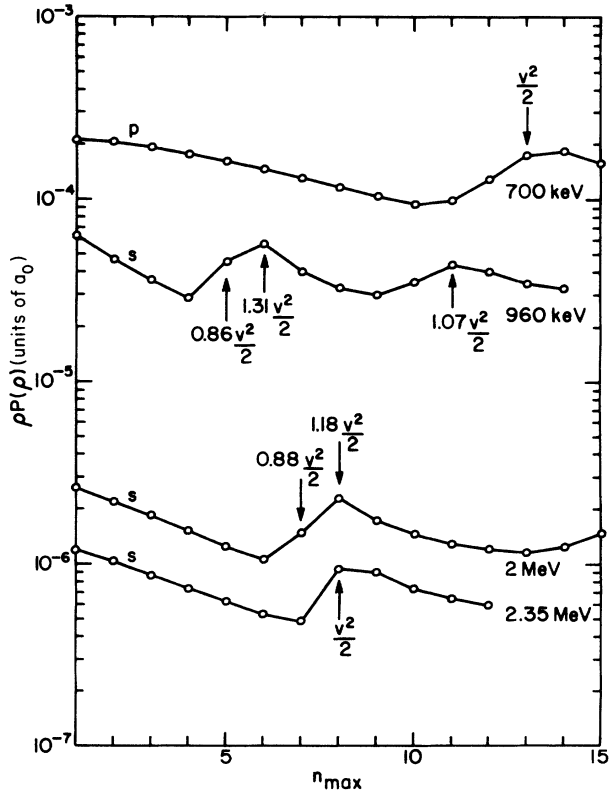

FIG. 4. Probability times impact parameter vs size of basis for electron transfer in proton-He^+ collisions. The Sturmian basis consists of 1s states centered on the proton and He^{2+}, plus ns or np states up to n_{max} on He^{2+}, as indicated. (In the case of the p curve, $n_{max}=1$ means that there are no p states.) The impact parameter is 0.25 for all curves, which are distinguished by proton energy $E=25v^2$ keV or type of basis. The peak in each curve occurs for the basis having an electronic state of positive-energy eigenvalue at or near $v^2/2$, as indicated.

fairly good agreement at both low and high energies (at least 21% for 30–50 keV and 28% for 1–2 MeV) is noteworthy. [In contrast, the two-state cross section (see Table I) is a factor of 2 too large by 2 MeV.] Thus the multistate Sturmian approach can account for the two-step (Thomas) mechanism. This will be explored in more detail in the following paragraphs.

The convergence of the high-energy Sturmian ionization cross section to the first-order Born value for a given partial wave, demonstrated in Sec. III A 2, does not guarantee that the specific continuum intermediate states needed for the two-step capture mechanism (Thomas mechanism) are included in the basis. In the two-step mechanism, the target electron is first promoted to a very high positive-energy state, of energy $v^2/2$, in order then to be captured by the proton moving at speed v. For a 2-MeV proton, this electronic energy is $+40$ a.u., which is much too high to contribute significantly to the ionization cross section. Indeed, most of the eigenvalues of the Sturmian basis are much less than this, unless the basis is very large, particularly for higher partial waves. However, for a given proton energy, as the target Sturmian basis of a particular l is enlarged, a basis function is occasionally formed having a positive-energy eigenvalue at or near $v^2/2$, further enlargement of the basis moving the eigenvalues away from $v^2/2$, until the process repeats. The effect of this on capture is seen clearly in Fig. 4 at a variety of proton energies and two different partial waves. For each of the four curves, and others not shown, the capture probability is enhanced about a factor of 2 by the presence of a $v^2/2$ basis function [22]. (Further, there are no stray peaks unconnected to $v^2/2$ functions.) The peaking does not require the function to have precisely the eigenvalue $v^2/2$; only $\frac{3}{5}$ of the displayed peaks do.

There is, however, sensitivity at small impact parameters to the particular enhancing basis when more than one is available. This was tested by using two different purely s bases corresponding to the two peaks in the 960-keV curve shown in Fig. 4 at $\rho=0.25$. The second peak is lower than the first, and the corresponding integrated cross section is lower by 15%. A 700-keV curve for purely s bases, not shown in Fig. 4, has three peaks of diminishing size as the basis is increased. Evidently, with a small basis, the isolation of a single $v^2/2$ function overly enhances the capture probability by flux trapping. As the basis is increased, the peaks appear to flatten and ap-

TABLE I. Sturmian cross sections for electron transfer and ionization in collisions between protons and $He^+(1s)$ ions at higher energies.

Proton energy (kev)	Total No. of Sturmians	Proton-centered Sturmians	He-centered Sturmians	Cross sections (10^{-18} cm^2) Ground state	All states	Ionization
225	35	$\leq 7s,3p$	$\leq 7s,8p,3d$	1.39	1.82	9.35
300	35	$\leq 7s,3p$	$\leq 7s,8p,3d$	0.50	0.72	8.01
	43[a]	$\leq 8s,4p$	$\leq 12s,8p,3d$		0.646	7.68
	51[a]	$\leq 8s,8p$	$\leq 12s,8p,3d$		0.623	7.92
450	25	$1s$	$\leq 7s,8p,3d$	0.109		4.30
	35	$\leq 7s,3p$	$\leq 7s,8p,3d$	0.09	0.13	7.30
482.5	35	$\leq 7s,3p$	$\leq 7s,8p,3d$	0.07	0.10	6.89
700	2	$1s$	$1s$	0.0332		0
	13	$1s$	$\leq 12s$	0.0246		0.43
	35′[b]	$1s$	$\leq 12s,12p$	0.0204		3.50
	65	$1s$	$\leq 12s,12p,12d$			<u>4.40</u>[c]
	26–35″	$1s$	$\leq 7-10s,10-13p$	<u>0.0192</u>		
750	51[a]	$\leq 8s,8p$	$\leq 12s,8p,3d$		0.015	4.66
960	2	$1s$	$1s$	0.008 25		0
	25–39	$1s$	$\leq 6-10s,10-15p$	<u>0.004 99</u>		
1000	13	$1s$	$\leq 12s$	0.005 05		0.31
	35′	$1s$	$\leq 12s,12p$	0.003 04		2.68
	65	$1s$	$\leq 12s,12p,12d$			<u>3.33</u>
	25′	$1s$	$\leq 7s,8p,3d$	0.0034		2.46
2000	2	$1s$	$1s$	0.000 231		0
	13	$1s$	$\leq 12s$	0.000 15		0.16
	35′	$1s$	$\leq 12s,12p$	0.000 08		1.55
	65	$1s$	$\leq 12s,12p,12d$			<u>1.89</u>
	25	$1s$	$\leq 7s,8p,3d$	0.000 11		1.42
	34	$1s$	$\leq 7s,8p,6d$	0.000 11		1.57
	37	$1s$	$\leq 7s,8p,7d$	0.000 11		1.63
	29–31	$1s$	$\leq 6-8s,12p$	<u>0.000 11</u>		

[a]The results of Stodden *et al.* [4].

[b]Different bases of the same size are distinguished by primes.

[c]The best of the present results are underlined.

proach a point midway between the peaks and adjacent valleys. Accordingly, it was decided to average the cross sections over the maxima and adjacent minima. The average cross sections obtained at 700 keV, 960 keV, and 2 MeV with these bases are the ones graphed in Fig. 3 and underlined in Table I. At 700 and 960 keV, both s and p peaks and valleys could be averaged out (average of four cross sections at each energy): At 700 and 960 keV, the s and p parts of the "peak bases" both have functions near $v^2/2$. At 2 MeV, on the other hand, although both s and p functions were included, the p basis could not be sufficiently enlarged to include such functions [23]; thus only s peaks and valleys could be averaged out (average of two cross sections).

The sensitivity to basis size is, not surprisingly, greater at smaller impact parameters $\rho \simeq 0.10$ at 960 keV corresponding classically to the scattering angle of the Thomas peak in the differential cross section at 0.47 mrad (if indeed it exists at this energy). It is premature here with a limited basis to attempt to determine the structure of the differential cross section. For a sufficiently large basis, it is expected that there would be greater stability as more states contribute to making a wave packet centered on $v^2/2$. Additional variational freedom could be attained within the Sturmian framework by choosing effective charges other than $Z=2$, following Shakeshaft for intermediate-energy p-H collisions [5].

Higher-angular-momentum states with $l \geq 2$ were not included in the bases used to determine the final high-energy capture cross sections. Test runs at 2 MeV show that d functions up to $7d$ affect the capture cross sections by at most a few percent. (See Table I.) It was not possible to include sufficiently many d Sturmians to create states of positive energy near $v^2/2$. It seems unlikely that their effect would be large: At least for direct ionization, d functions are important only for larger impact parameters, whereas capture takes place at smaller impact parameters.

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