PHYSICAL REVIEW A, VOLUME 61, 052709

Ionization in collisions between (200–2000)-keV protons and He^+(1s, 2s, or 3s) ions studied using a Sturmian basis

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(Received 14 December 1999; published 10 April 2000)

Cross sections have been determined for ionization as well as stripping in collisions between protons and He^+ ions in the 1s, 2s, or 3s state for proton energies from 200 keV to 2 MeV using the coupled-Sturmian-pseudostate approach. Detailed convergence studies are presented. For comparison, and to include neglected higher partial waves, first Born cross sections are also reported. By using a larger basis, this work extends earlier calculations that were limited to the 1s initial state [T. G. Winter and S. G. Alston, Phys. Rev. A **45**, 1562 (1992)]. Further, a correction has been applied to the uneven distribution of Sturmian-generated energies at the ionization threshold, yielding cross sections much more stable with respect to basis size.

PACS number(s): 34.50.Fa

I. INTRODUCTION

Ionization, as well as electron transfer, in collisions between protons and He^+ ions in the ground state has been of considerable interest both theoretically and experimentally for more than two decades. In the past decade, several calculations have been reported on this basic asymmetric collisional system and, of these, the coupled-state approaches are potentially the more reliable over the largest range of energies. Extensive coupled-Sturmian-pseudostate calculations were reported in 1990 by Stodden *et al.* [1] and, two years later, by Winter and Alston [2], the latter authors focusing on higher energies. More recently, Henne *et al.* [3] proposed and applied a doorway approximation [3] of the time-dependent optical potential and Errea and Sánchez [4] employed a similar coupled-state approach including probability-absorber or doorway states, while Errea *et al.* [5] used a coupled-molecular-state approach with pseudostates. Hose [6] and Brown and Crothers [7] also considered the same collisional system, but for electron transfer only. The largest basis calculation was the single-center calculation of Hall, Reading, and Ford [8]. These theoretical works on ionization and electron transfer from the ground state also cited earlier theoretical results. The most recent experiments were carried out by Watts *et al.* [9] and Rinn *et al.* [10], but only the earlier measurements of Angel *et al*. [11] extended into the presently considered higher energy range.

Hall *et al.* [8] also reported coupled-state results for $n=2$ initial states. There are no other coupled-state results for $n=2$ initial states, and none for more highly excited initial states. There are no experimental results for any excited initial state.

These collision processes are not only fundamental but also relevant to understanding nuclear fusion. In muon-catalyzed fusion, 23% of $\alpha\mu$ ions are in an excited state following fusion [12], and the stripping (transfer or ionization) cross section in part determines the extent to which muons are available to catalyze subsequent fusions [13]. This cross section may be scaled to that with electrons rather than muons [13]. Of particular interest are p-He^+ collisions in which the relative velocity is about $5\text{a.u.}=1.09\times10^7$ m/s [14], corresponding to a proton energy of 625 keV; the highest relevant speed is that of an $\alpha\mu$ ion following fusion, 5.83 a.u. [13].

The present article considers the process of stripping from the 1s, 2s, or 3s states and encompasses the intermediate and higher proton energies 200–2000 keV; at these energies, stripping and ionization will be seen to be almost synonymous.

This work extends the coupled-Sturmian-pseudostate calculations of Refs. [1,2] to the 2s and 3s initial states. In addition, the ground-state process has also been re-examined with a larger, more systematically varied basis and with attention to a correction for the uneven distribution of pseudostate eigenvalues at the ionization threshold. For each initial state, the results can be benchmarked against the Born approximation at sufficiently high energies, and the energy range of validity of the Born approximation can also be delineated.

The outline of the paper is as follows. In Sec. II, the Sturmian approach will be summarized and the threshold correction described. In Sec. III, the convergence of cross sections with respect to basis size will be presented in detail using the Born values as reference points, and the largest-basis results will be compared with other available coupled-state results and experimental results. Atomic units are used except where otherwise noted.

II. METHOD

A. Background

Sturmians were introduced in atomic (specifically, elastic e-H and e^+-H) scattering theory by Rotenberg in 1962 [15]. Six years later, Gallaher and Wilets carried over the coupled-Sturmian approach to ion-atom (p-H) scattering [16]. In the early 1970's, Reinhardt, Oxtoby, and Rescigno [17], and coworkers successfully applied the Sturmian, or fixed-exponent-Laguerre, basis to e-H (and other e-atom) scattering, while a little later Shakeshaft [18] made several innovations working on p-H collisions. The fixed-exponent basis was also applied at that time to e-H_2 scattering by Winter and Lane [19] in a limited calculation. In 1982, Winter extended the Sturmian approach to asymmetric ion-atom (specifically, p-He$^+$ and He^{2+}-H) collisions [20] and later to other systems [21]. In the early 1990s, Bray and Stelbovics [22] and co-workers began extensive, highly successful Sturmian calculations, first on e-atom scattering with H targets, and later with many other targets. There have thus been two parallel, somewhat disjoint approaches, one applied to e-atom scattering and the other to ion-atom scattering.

The setup of the computational formalism used by Winter in ion-atom collisions may be found in Ref. [20], and present numerical details are, for the most part, as in Ref. [21], except for the threshold correction to be described in the next section. Whether applied to collisions for which the projectile is an electron or an ion, the radial Sturmian basis functions are simply exponentials e^{-cr} multiplied by polynomials in the radial variable r, with c being *fixed* for a given angular momentum l. Since the polynomials form a complete set, the Sturmians do as well. (For a large, two-center basis, the set is overly complete.) In most of Shakeshaft's and Winter's work, c is taken to be $Z/(l+1)$, where Z is the nuclear charge of a particular center. If the initial state is the ground state (or $2p$,$3d$, etc.), this ensures that the initial state can be represented by a single Sturmian. For simplicity and programming convenience, this is also done in the present work, even though other considered initial states, particularly $3s$, will be seen to require many more Sturmians to represent them.

Following Rotenberg [15], Gallaher and Wilets [16], and Shakeshaft [18], Winter has employed orthogonal Sturmians with $1/r$ (i.e., potential) weighting, while those of Bray and Stelbovics are orthogonal without this weighting factor. Although the former set may be somewhat less well conditioned in very large calculations of limited accuracy, both sets span the same space. To test for numerical difficulties with the present pseudostate basis of up to principal quantum number $n=18$ (larger than used in the past by Winter) for each l, energy eigenvalues have been computed using both the existing FORTRAN program and MATHEMATICA; the results are the same to eight digits. In summary, it has not proven necessary to modify the computer program to incorporate the alternate weighting factor for the Sturmian bases used here.

B. Threshold correction

Let ϵ_i, $i=1,\ldots,N$, be the Sturmian-generated eigenvalues of the He$^+$ Hamiltonian for a given angular momentum l, and let $P(\epsilon_i)\equiv P_i$ be the probability of a transition to the ith pseudostate obtained by solving the coupled-scattering equations at a given impact parameter ρ and proton energy E. The (electronic) energy-differential transition probability for the interval $\Delta\epsilon_i\equiv\epsilon_{i+1}-\epsilon_i$ is [23]

$$\frac{dP(\overline{\epsilon_i})}{d\epsilon}\cong\frac{1}{2}\,\frac{P_i+P_{i+1}}{\Delta\epsilon_i}.$$

Suppose $\epsilon_n<0$ and $\epsilon_{n+1}>0$. Then the correct contribution to the ionization probability from the ionization threshold to $\epsilon_{n+1}$is approximately

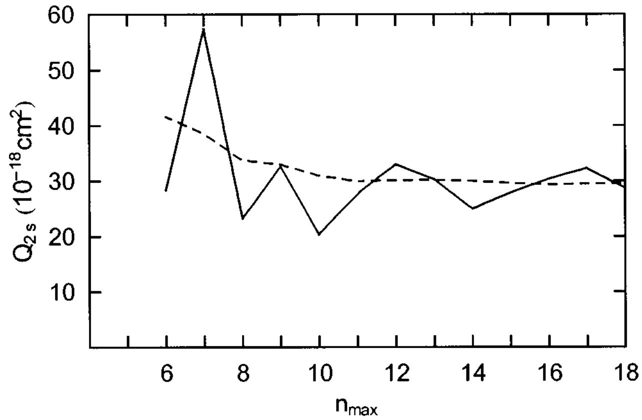

FIG. 1. Cross sections for ionization in collisions between 200-keV protons and He$^+(2s)$ ions versus size of the Sturmian basis $1s_{\rm H},\leq n_{\rm max}(s,p)_{\rm He}$ without (solid line) and with (dashed line) a correction at the ionization threshold.

$$\left[\frac{dP(\overline{\epsilon_n})}{d\epsilon}\Delta\epsilon_n\right]\left(\frac{\epsilon_{n+1}-0}{\Delta\epsilon_n}\right).$$

Previously, the total ionization probability was obtained simply as

$$P_{\rm total}=\sum_{i=n+1}^{N}P_i=\frac{1}{2}\,\frac{P_{n+1}}{\Delta\epsilon_n}\Delta\epsilon_n+\sum_{i=n+1}^{N-1}\frac{dP(\overline{\epsilon_i})}{d\epsilon}\Delta\epsilon_i+\frac{1}{2}P_N.$$

Thus a correction

$$\delta P=\frac{dP(\overline{\epsilon_n})}{d\epsilon}\Delta\epsilon_n\left(\frac{\epsilon_{n+1}-0}{\Delta\epsilon_n}\right)-\frac{1}{2}\,\frac{P_{n+1}}{\Delta\epsilon_n}\Delta\epsilon_n$$
$$=\frac{1}{2}\,\frac{P_n\epsilon_{n+1}+P_{n+1}\epsilon_n}{\epsilon_{n+1}-\epsilon_n}$$

must be added to $P_{\rm total}$. This correction is not necessarily small if $\epsilon_n\neq-\epsilon_{n+1}$. Bray and Fursa [24] have also been aware of the possible need to include a contribution from negative-energy states in considering *electron*-impact ionization of atoms, but they have noted that the correction is generally small when the basis is large enough. We have found the correction often to be quite significant, particularly for the s,p-state contributions to the total ionization cross section.

As an example of the improvement with this threshold correction, cross sections are shown in Fig. 1 without and with the correction for ionization in 200-keV p-He$^+(2s)$ collisions obtained with coupled-Sturmian-pseudostate bases $1s_{\rm H},\leq n_{\rm max}(s,p)_{\rm He}$, where $n_{\rm max}$ varies from 6 to 18. It is seen that the very large, oscillatory basis sensitivity is smoothed by the threshold correction [25].

III. RESULTS

A. First Born approximation

The high energy limit of the ionization cross section is given by the first Born approximation. For an initial $1s$ state,

TABLE I. Present first Born cross sections (10^{-18} cm^2) for the three lowest partial waves $l=0,1,2$ for ionization in $p+He^+(1s,\ 2s,$ or $3s)$ collisions at various proton energies E.

Initial state	l	E (keV) 200	500	1000	2000
1s	0	1.36	0.622	0.322	0.164
1s	1	6.47	3.96	2.45	1.45
1s	2	2.58	1.42	0.775	0.402
2s	0	5.71	2.37	1.20	0.601
2s	1	22.7	12.6	7.59	4.42
2s	2	7.11	2.99	1.52	0.764
3s	0	12.0	4.88	2.45	1.23
3s	1	46.3	24.6	14.5	8.27
3s	2	17.1	6.89	3.46	1.73

integrated Born cross sections have been calculated and plotted by Bates and Griffing [26] for collisions between protons and hydrogen atoms. These cross sections can be scaled to collisions between protons and ions such as He^+ [27]. For the 1s, 2s, and 3s as well as other initial states, Igarashi and Shirai [28,29] have determined cross sections for hydrogenic targets such as He^+ using the continuum-distorted-wave, eikonal-initial-state (CDW-EIS) approach. These cross sections may be expected to agree with the first Born results at high energies and improve on them at lower energies.

In a coupled-state approach such as that reported here, ionization probabilities are calculated one impact parameter ρ at a time and, except for an intractably large basis, are limited to the dominant lower partial waves l. For the sake of a detailed comparison with their coupled-state results for an initial 1s state, Winter and Alston [2] calculated the first-order Born ionization probability for one value of l and ρ at a time. Summed over l and integrated over ρ, these results could then also be checked explicitly against the scaled cross sections of Bates and Griffing.

The Winter-Alston Born calculations have now been extended to the 2s and 3s initial states, necessitating the inclusion of additional partial waves. Following Winter and Alston, the calculation is carried out using the formulas for the Coulomb wave function and auxiliary functions in Bethe and Salpeter [30] and Abramowitz and Stegun [31]. The ionization probability for each l and ρ has been obtained by integrating numerically over the radial electronic coordinate, collision time, and continuum electronic energy. This procedure is also followed here, but to a generally higher degree of accuracy: For the 1s, 2s, and 3s initial states, it is estimated that the Born partial cross sections up to $l=8$ are numerically accurate to at least 0.1%, 0.1%, and 1%, respectively.

For later comparison with s,p,d-state ionization cross sections, s,p,d-wave Born cross sections are given in Table I. The p partial wave contributes 55–64 %, 35–51 %, and 31–45 % to the total Born ionization cross section for 1s, 2s, and 3s initial states, respectively, and this contribution increases with increasing energy over the studied proton energy range 200–2000 keV. In the Winter-Alston Born calculation for the 1s initial state, only the lowest five partial waves were included. For this initial state, these partial waves contribute 98–97 % to the total cross section, while for the 2s and 3s initial states, the corresponding contributions are only 83–87 % and 67–74 %, respectively. Including also the next four partial waves (i.e., $l=0-8$ in all) brings the contribution to 99.9–99.5 %, 96.8–97.5 %, and 93–94 % for the three respective initial states over the energy range 200–2000 keV. The extrapolated contribution from partial waves $l>8$ has been estimated by assuming they form a geometric sequence [32].

TABLE II. First Born (present, scaled Bates and Griffing [26]) and CDW (Igarashi [29]) cross sections (10^{-18} cm^2) for ionization in $p+He^+(1s,\ 2s,$ or $3s)$ collisions at proton energies E.

Initial state	Authors	E (keV) 200	500	1000	2000
1s	Present	11.7	6.85	4.03	2.265
1s	Bates and Griffing	11.7	6.9	4.0	2.2
1s	Igarashi	12.1	6.89	3.99	2.23
2s	Present	64.4	29.6	16.2	8.71
2s	Igarashi	63.0	29.4	16.1	8.74
3s	Present	148	65.7	35.5	18.6
3s	Igarashi	148	66.6	36.2	19.1

Shown in Table II are the present first Born ionization cross sections along with the scaled Born ionization cross sections of Bates and Griffing [26] for the 1s initial state and the CDW-EIS results of Igarashi [29] for the three initial states. For the 1s initial state, the present Born results agree closely (within 1.6%) with the graphical cross section of Bates and Griffing over the full energy range and also (within 1%) with the CDW-EIS results at proton energies of at least 500 keV; at 200 keV, the CDW-EIS result is 3% *higher* and would have been assumed to be a slight improvement over the Born value except that the coupled-state cross section will be seen to be somewhat *below* the Born cross section. For the 2s initial state, the present Born and CDW-EIS results agree very closely (within 0.8%) at proton energies of at least 500 keV. At 200 keV, the CDW-EIS result is only 2% *lower*, while the coupled-state result will be seen to be slightly *above* the Born cross section. For the 3s initial state, the difference between the CDW-EIS result and the present Born result increases from 0.5% to 2.8% as the proton energy increases from 200 to 2000 keV. The small difference at higher energies is unphysical and probably reflects a small numerical inaccuracy in either of the calculations; a possible source of error in the present calculation is in the estimate of the non-negligible contribution from partial waves $l>8$ for this higher initial state [32].

Not shown are the first-Born results of Hall *et al.* [8] for the 1s and 2s initial states, which can be inferred from their tabulated percent differences of their coupled-state results from their Born results (not explicitly given). For the 1s and 2s initial states, their Born values are respectively 1–3 % and 10% below the present Born results in the overlapping energy range of 200–500 keV.

The high energy limit of the Born approximation is obtained in the Bethe approximation [33] as $Q=a\ln(BE)/E$

$=a(\ln E+b)/E$, where E is the proton's energy. Using the present Born values in Table II at $E=1$ and 2 MeV to determine the constants a and b, we obtain the two-term fit

$$Q_{1s}^{\mathrm{Bethe}}=\frac{1.03}{v^2}[\ln(v^2)+1.92]a_o^2,$$

where $v=\sqrt{E(\mathrm{keV})/25}$ is the proton's speed in atomic units and a_o is the Bohr radius. Compare Cohen's three-term fit [34]:

$$Q_{1s}^{C}=\frac{0.90}{v^2}\left[\ln(v^2)+3.03-\frac{8.0}{v^2}\right]a_o^2.$$

This fit gives values within 2% of the present Born cross sections at 1–2 MeV. Both fits lie 3% above the present Born values at 500 keV. Cohen's fit agrees more closely with the Born value at 200 keV than does the Bethe fit (+10% versus +23%), but the Born approximation itself will be seen not to be very reliable at this ''intermediate energy.'' (On the other hand, at high energies of 3–20 MeV, the two fits agree to within 1%.)

For higher excited states, the two-term (Bethe) fit can be written in a similar form:

$$\frac{Q_{ns}^{\mathrm{Bethe}}}{n^4}=\frac{a_{ns}}{(nv)^2}[\ln(nv)^2+b_{ns}],$$

where

$$a_{2s},b_{2s}=0.654,3.75,$$

$$a_{3s},b_{3s}=0.372,9.24$$

using the present Born values in Table II at $E=1$ and 2 MeV to determine the constants a_{ns},b_{ns}. For the $2s$ state, the Bethe fit lies above the present Born values by 0.5% and 2.6% at $E=500$ and 200 keV, respectively, whereas for the $3s$ state the agreement is only to within 3% and 7%. The n^4 scaling with principal quantum number n is obeyed classically [34–37]; however, in view of the dependence of the coefficients a_{ns},b_{ns} and of the graphs of Q/n^4 versus nv (not shown) on n, this scaling for small values of n holds only qualitatively in the Born approximation; compare Olivera *et al.* [37] on p-H(n) ionization also using the Born approximation (where n denotes a principal quantum *shell*).

B. Convergence with coupled Sturmian basis

1. Role of projectile-centered states

Ionization dominates electron transfer and is described by the first Born approximation at high energies. Therefore, only target-centered basis functions are expected to be important to describe it at sufficiently high energies. In the present calculation, a fairly large target-centered basis has been used, augmented by a single projectile-centered state to describe any residual effect of electron transfer on the ionization cross section. To test the importance of this state, calculations have been performed with the target-centered states $\leqslant 11(s,p,d)_{\mathrm{He}}$, with and without the projectile-centered function $1s_{\mathrm{H}}$. For ionization from a $1s$ initial state, the presence of this function *decreases* the ionization cross section by 14%, 6%, and 2% at the proton energies 200, 300, and 500 keV, respectively. The effect at a given energy is smaller when the initial state is excited: For a $2s$ initial state, the effect is -3.8% and -0.3% at 200 and 500 keV, respectively, while for the $3s$ state, the corresponding effect is -0.7 and $<0.1\%$. At 1 or 2 MeV, the effect is $\leqslant 0.1\%$ for all three initial states. When not negligible, the effect is primarily due simply to the loss of flux to the open electron-transfer channel rather than indirect coupling. In these cases one could multiply the effect by a factor of 1.2 to allow for neglected excited electron-transfer channels, but the results reported here—all of which include $1s_{\mathrm{H}}$ in the basis—do not contain this additional correction.

2. Role of target-centered states

(a) s states. Partial-wave Born cross sections are a convenient reference point for coupled-state cross sections and, at high energies, a benchmark. Shown in Fig. 2 are differences from s-wave Born cross sections of ionization cross sections obtained with a purely s-state basis $\leqslant n_{\max}s_{\mathrm{He}}$ (as well as $1s_{\mathrm{H}}$) for $1s$, $2s$, and $3s$ initial states. All values reported in this and the following sections are corrected for the uneven distribution of Sturmian-generated electronic energies at the ionization threshold as in Sec. II B. It is seen that, to achieve convergence, the more excited the initial state, the larger the basis needed, but also that the Born limit sets in at lower proton energies. For the $1s$ initial state, the converged limit is significantly different from the Born cross section at the lowest proton energy, 200 keV. In the converged limit, the s-state cross section is below the corresponding Born value by 12%, 4%, 1%, and 0.6% at proton energies of 200, 500, 1000, and 2000 keV, respectively, and this converged coupled-s-state limit is achieved to within an accuracy of $\approx 0.5\%$ using $\approx 10s$ states. (Note, on the other hand, that with too small a basis, even the sign of the difference is wrong at most energies.) For the $2s$ initial state, the difference from the Born cross section using the largest basis is 1–3 % over the full energy range, while for the $3s$ state it is 24–25 %, and for either state the difference does *not* decrease with increasing energy. For $3s$, the large difference indicates that the s-wave ionization cross section is not converged. However, as will be seen, this partial wave has only a small effect on the summed cross section.

Is the need for a large s-state basis dictated by the need for higher-lying positive-energy pseudostates in the basis? This question is answered by referring to Fig. 3, which shows differences from s-wave Born cross sections of cross sections obtained with the bases $\leqslant \overline{n_{\max}s_{\mathrm{He}}}$ (plus $1s_{\mathrm{H}}$) formed from the basis $\leqslant 18s_{\mathrm{He}}$. Here the overline refers to hydrogenic pseudostates formed by diagonalizing the He^{+} Hamiltonian in the largest s-state Sturmian basis, $\leqslant 18s_{\mathrm{He}}$. For example, the basis $\leqslant \overline{17s_{\mathrm{He}}}$ has the highest-lying pseudostate $\overline{18s_{\mathrm{He}}}$ removed. For the $1s$ initial state, the *two* highest-lying pseudostates each affect the ionization cross section by

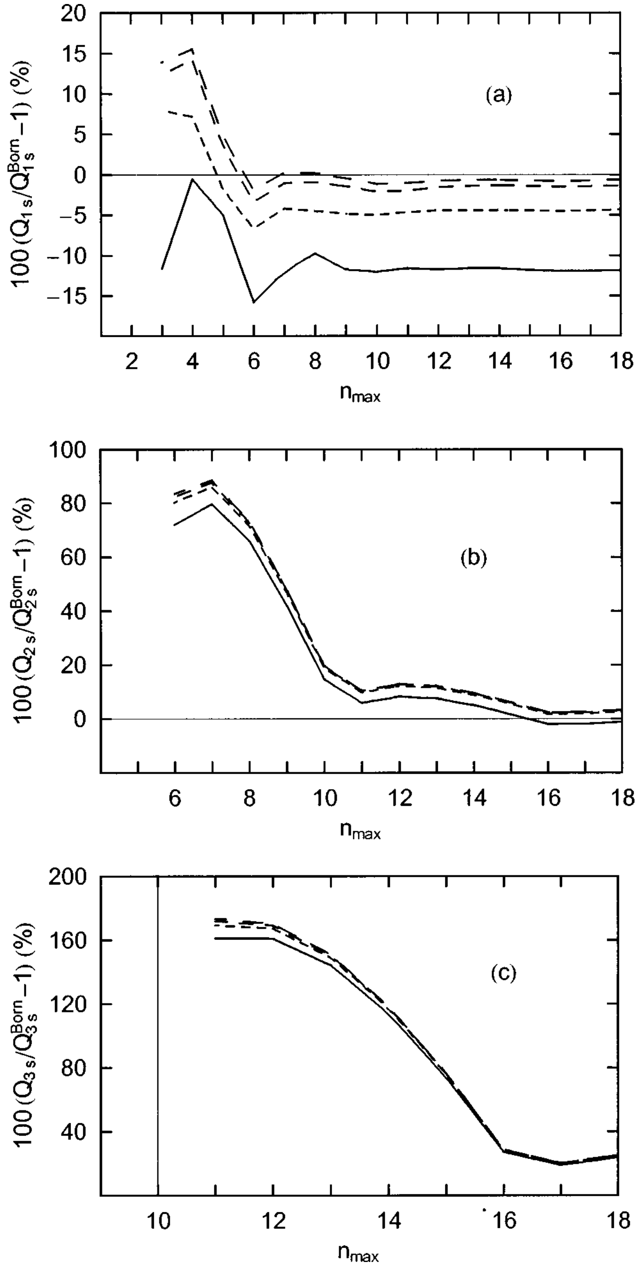

FIG. 2. Percent differences from s-wave Born cross sections $Q^{\rm Born}$ of Sturmian cross sections Q versus size of the Sturmian basis $1s_{\rm H}, \leqslant n_{\rm max}s_{\rm He}$ for p-$\rm He^+$ ionization at the proton energies 200 keV (solid line), 500 keV (short dashes), 1000 keV (longer dashes), and 2000 keV (longest dashes). (a) $1s$ initial state. (b) $2s$ initial state. (c) $3s$ initial state.

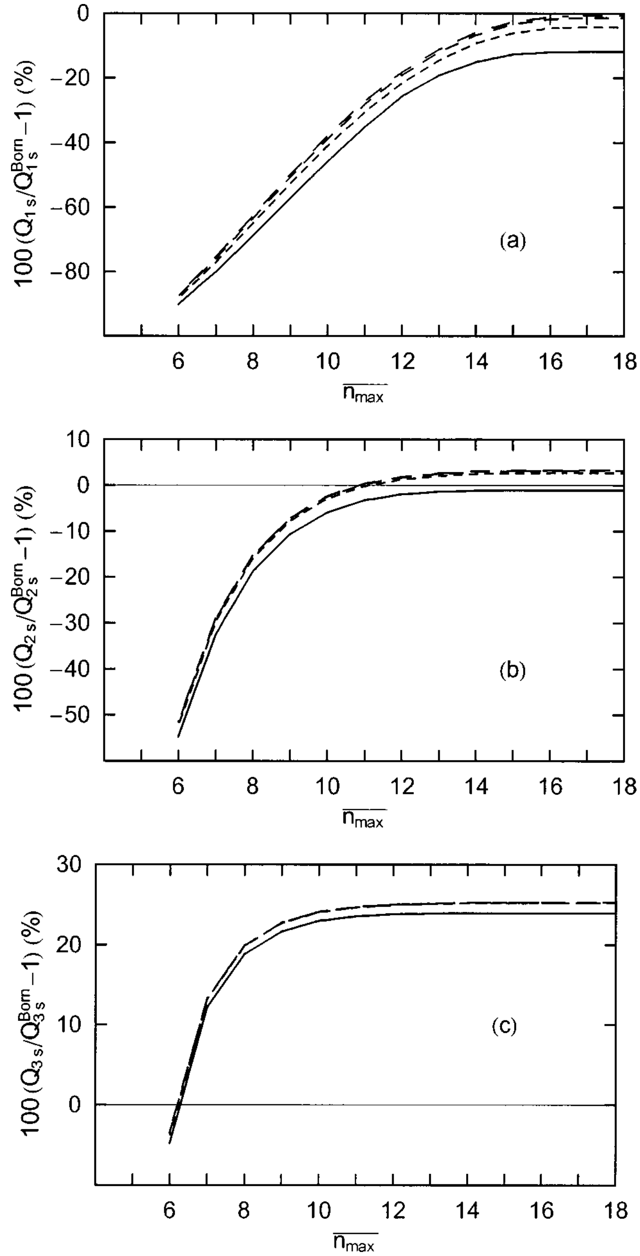

FIG. 3. Percent differences from s-wave Born cross sections $Q^{\rm Born}$ of Sturmian cross sections Q versus size of the Sturmian basis $1s_{\rm H}, \leqslant \overline{n}_{\rm max}s_{\rm He}$ for p-$\rm He^+$ ionization at proton energies 200 keV (solid line), 500 keV (short dashes), 1000 keV (longer dashes), and 2000 keV (longest dashes). (a) $1s$ initial state. (b) $2s$ initial state. (c) $3s$ initial state. The basis used to determine the pseudostates $\leqslant \overline{n}_{\rm max}s$ by diagonalizing the $\rm He^+$ Hamiltonian is $\leqslant 18s$.

$\leqslant 0.5\%$ at any proton energy. For the $2s$ initial state, the *five* highest states and, for the $3s$ initial state, the *eight* highest states have only this small effect. That is, for the $1s$ initial state, a large Sturmian basis is not required, as seen in the preceding paragraph, but once it is formed, only two pseudostates, $\overline{17s}_{\rm He}$ and $\overline{18s}_{\rm He}$, may be removed from the basis after diagonalization for 0.5% accuracy. On the other hand, for the $3s$ initial state, a large s-wave basis of at least 18 Sturmians is required, but once it is formed, many pseudostates may be removed. The large basis is required to some extent to *define* the initial state, since the exponent in the radial s Sturmian functions used here is $-Zr$ rather than the correct $-\frac{1}{3}Zr$ ($Z=2$ being the target nuclear charge) for the $3s$ state. However, little ionization flux is carried away by higher lying pseudostates obtained by diagonalizing the $\rm He^+$ Hamiltonian; removing these higher-lying states is thus justified and could considerably reduce computing time, but this has not been done here.

(b) s and p states. Shown in Fig. 4 are differences from s,p-wave Born cross sections of ionization cross sections

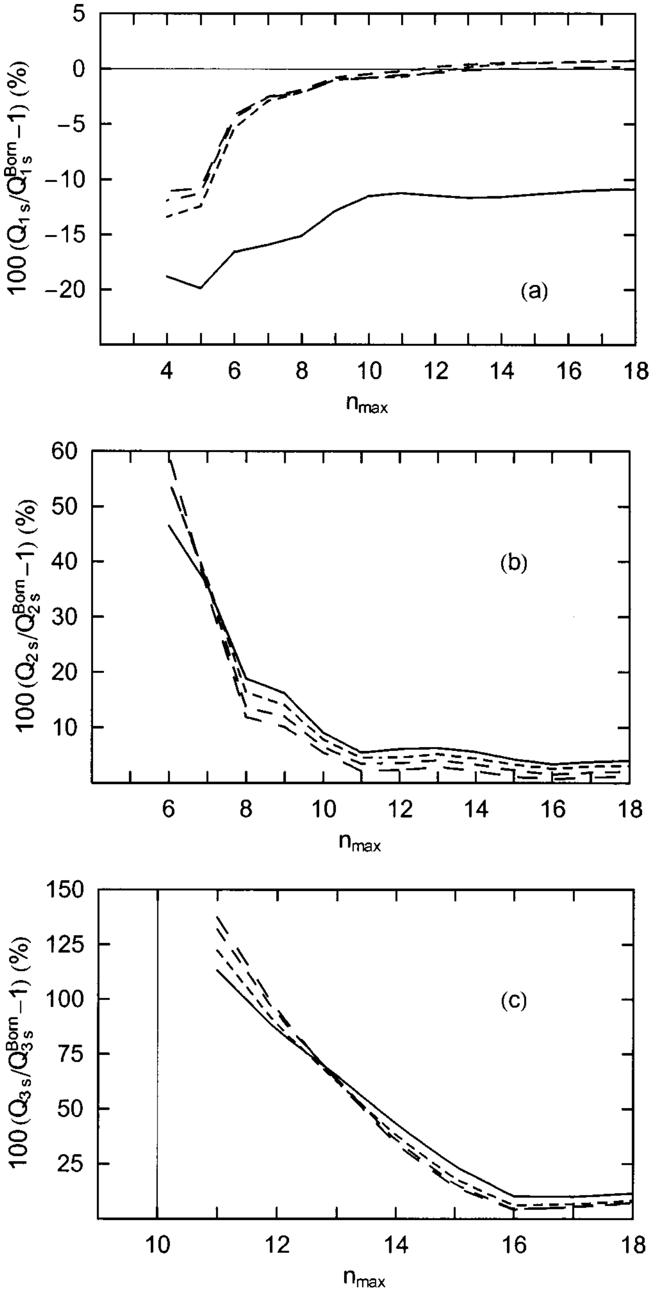

FIG. 4. Percent differences from s,p-wave Born cross sections Q^{Born} of Sturmian cross sections Q versus size of the Sturmian basis $1s_{\mathrm{H}}, \leqslant n_{\max}(s,p)_{\mathrm{He}}$ for p-He^{+} ionization at proton energies 200 keV (solid line), 500 keV (short dashes), 1000 keV (longer dashes), and 2000 keV (longest dashes). (a) $1s$ initial state. (b) $2s$ initial state. (c) $3s$ initial state.

obtained with a purely s,p-state bases $\leqslant n_{\max}(s,p)_{\mathrm{He}}$ (as well as $1s_{\mathrm{H}}$) for $1s$, $2s$, and $3s$ initial states. Qualitatively, the same conclusions hold as for an s-state basis: To achieve convergence, it takes a larger basis, but the Born limit sets in at lower energies, the more excited the initial state is. The converged limit is significantly different from the Born cross section at the lowest energy, 200 keV, for the $1s$ initial state: The largest-basis s,p-state cross section differs from the corresponding Born value by -11%, $+0.7\%$, 0.8%, and 0.2% at proton energies of 200, 500, 1000, and 2000 keV, respectively, and the converged coupled-state limit is achieved to within an accuracy of 1% with the basis $\leqslant 10(s,p)_{\mathrm{He}}$. For the $2s$ initial state, the difference of the largest s,p-basis result from the Born cross section is $+4\%$, 3%, 2%, and 1% at proton energies of 200, 500, 1000, and 2000 keV, respectively, while for the $3s$ state it is $+12\%$, 8%, 7%, and 7% at corresponding energies. These differences from the partial-wave Born cross section are generally smaller than those for s waves only, significantly smaller in the case of a $3s$ initial state, for which the 7–8 % difference at the higher energies probably reflects the extent of basis nonconvergence rather than a failing of the Born approximation.

Could the s,p basis be reduced after diagonalizing the He^{+} Hamiltonian by removing some of the higher-lying $\overline{p}$ pseudostates, as well as $\overline{s}$ pseudostates, as might have been done for the purely s-state basis of the preceding section? The answer is that there are fewer higher-lying $\overline{p}$ pseudostates, so less is to be gained.

(c) s, p, and d states. To include d states as well in the Sturmian basis, two approaches have been taken. First, these states have been fully coupled to the s and p states. However, the present program limited this calculation to at most the 59 Sturmians $1s_{\mathrm{H}}, \leqslant 11(s,p,d)_{\mathrm{He}}$. To extend the basis further, a second approach has been taken. Following Winter and Alston, the d ionization cross section was merely added to the fully coupled s,p cross section: the d states were coupled only to $1s_{\mathrm{H}}$ and $\overline{s}_{\mathrm{He}}$ pseudostates up to the initial state $\overline{ns}$—i.e., the bases $1s_{\mathrm{H}}$, $\leqslant(\overline{ns}, n_{\max}d)_{\mathrm{He}}$. In this basis, the $\overline{2s}$ and $\overline{3s}$ pseudostates here have originally been obtained by diagonalizing the He^{+} Hamiltonian with the limited basis $\leqslant 12s$, which is not very accurate for $\overline{3s}$; the final form, $\overline{3s'}$, used in the next section is obtained with the basis $\leqslant 17s$. Shown in Fig. 5 for only the $ns=1s$ and $2s$ initial states are differences from s,p,d-wave Born cross sections of ionization cross sections with fully coupled s,p,d states, and shown in Fig. 6 for the $ns=1s$, $2s$, and $3s$ initial states are differences from s,p,d-wave Born cross sections of ionization cross sections obtained by adding cross sections with the *separate* bases $1s_{\mathrm{H}}, \leqslant n_{\max}(s,p)_{\mathrm{He}}$ and $1s_{\mathrm{H}}, \leqslant(\overline{ns}, n_{\max}d)_{\mathrm{He}}$.

For the $1s$ initial state, as the fully coupled s,p,d basis is increased, the differences from the s,p,d-wave Born cross section in Fig. 5(a) decrease in magnitude monotonically to 2–4 % using the largest, 59-state basis $1s_{\mathrm{H}}, \leqslant 11(s,p,d)_{\mathrm{He}}$ over the full energy range. For this same initial state, as the *separately* coupled s,p,d basis is increased, the differences from the Born cross section in Fig. 6(a) also decrease in magnitude monotonically, here to 15% at 200 keV and $\leqslant 0.9\%$ at $E \geqslant 500$ keV with the largest, ‘‘101-state’’ separately coupled basis $1s_{\mathrm{H}}, \leqslant 18(s,p,d)_{\mathrm{He}}$ as described above. The coupled-state cross sections with both types of bases are *below* the Born cross section at all energies. With the exception of the lowest energy, the separately coupled basis has smaller differences from the Born cross section than does the fully coupled basis, owing to its greater size, and may be considered more fully converged. Cross sections with the same size basis, the fully coupled 59-state and the separately

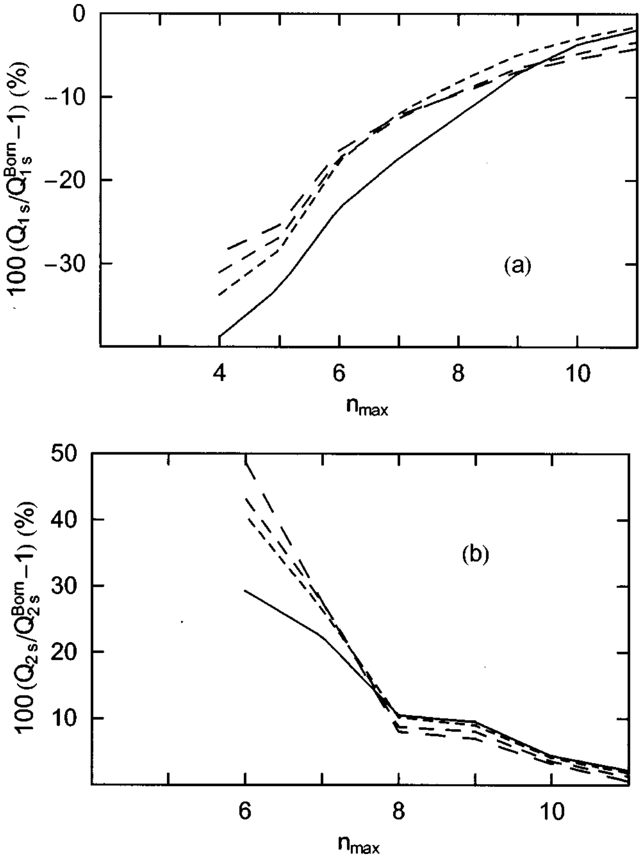

FIG. 5. Percent differences from s,p,d-wave Born cross sections Q^{Born} of Sturmian cross sections Q versus size of the Sturmian basis $1s_{\mathrm{H}},\leqslant n_{\max}(s,p,d)_{\mathrm{He}}$ for p-He^{+} ionization at the proton energies 200 keV (solid line), 500 keV (short dashes), 1000 keV (longer dashes), and 2000 keV (longest dashes). (a) $1s$ initial state. (b) $2s$ initial state.

coupled ''59-state'' bases, differ by only 0.4% at the highest energy. The situation at the lowest energy is unclear: Results with the same size bases differ by 15%. The cross section with the largest ''101-state'' basis, $1s_{\mathrm{H}},\leqslant 18(s,p,d)_{\mathrm{He}}$, has been noted to be 15% below the Born result, while that with the largest fully coupled 59-state basis, $1s_{\mathrm{H}}$, $\leqslant 11(s,p,d)_{\mathrm{He}}$, is only 2% below the Born result. Since the Born cross section may not be reliable at this ''intermediate energy,'' the ''101-state'' result, having the larger difference from the Born value, may in fact be the better one. In the next section, when coupled-state results are compared with those of others, two sets of coupled-Sturmian results are given if it is not clear which one is better.

For the $2s$ initial state, as the fully coupled s,p,d basis is increased, the differences from the s,p,d-wave Born cross section in Fig. 5b decrease to +2.2%, 1.8%, 1.3%, and 0.6% at energies of 200, 500, 1000, and 2000 keV, respectively, with the largest 59-state basis, $1s_{\mathrm{H}},\leqslant 11(s,p,d)_{\mathrm{He}}$. For this same initial state with separate s,p, and d coupling, cross sections with the largest ''95-state'' basis, $1s_{\mathrm{H}}$, $\leqslant 17(s,p,d)_{\mathrm{He}}$, differ from the Born cross sections in Fig. 6(b) by +1.2%, 1.9%, 1.2%, and 0.6% at these respective energies. For $E\geqslant 500$ keV, the almost identical differences from the Born cross sections with either of the two largest

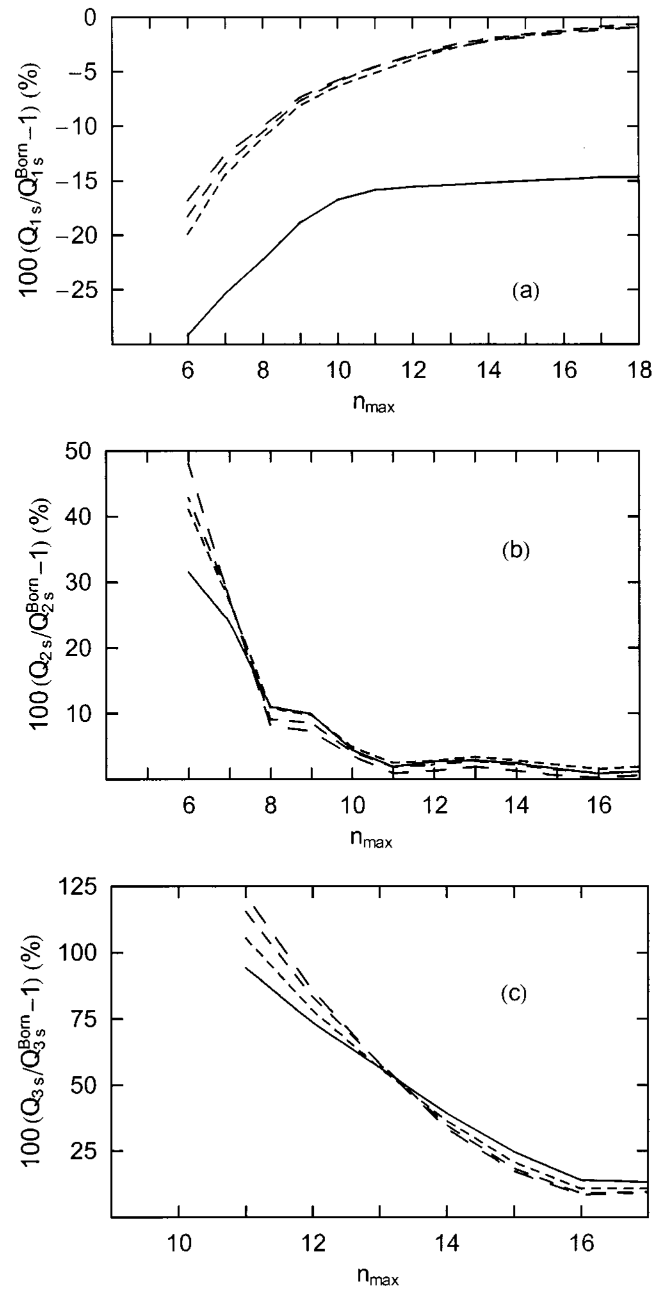

FIG. 6. Percent differences from s,p,d-wave Born cross sections Q^{Born} of Sturmian cross sections Q versus size of the two separately coupled Sturmian bases $1s_{\mathrm{H}},\leqslant n_{\max}(s,p)_{\mathrm{He}}$ and $1s_{\mathrm{H}}$, $\leqslant(\overline{ns},n_{\max}d)_{\mathrm{He}}$ for p-He^{+} ionization at proton energies 200 keV (solid line), 500 keV (short dashes), 1000 keV (longer dashes), and 2000 keV (longest dashes). (a) $\overline{ns}=1s$ initial state. (b) $\overline{ns}=2s$ initial state. (c) $\overline{ns}=3s$ initial state. Here the basis used to determine the pseudostates $\leqslant\overline{ns}$ by diagonalizing the He^{+} Hamiltonian is $\leqslant 12s$.

bases may reflect a small but real improvement over the Born approximation. Cross sections with the same size basis, the fully coupled 59-state and the separately coupled ''59-state'' bases, differ by only 0.4% at the highest energy, as for the $1s$ initial state, and by at most 0.7% at any energy. Indeed, the two sets of results differ only slightly for all bases of the same size.

TABLE III. Coupled-state and Born-extrapolated cross sections (10^{-18} cm^2) for ionization and stripping in $p+\mathrm{He}^+(1s)$ collisions at various proton energies E.

E (keV)	Number of functions	Proton center	Helium center	Ionization: Coupled state	Ionization: Born ext	Ionization: Coupled state +Born	Electron transfer	Stripping: Coupled state +Born
200	59	$1s$	$\leqslant 11(s,p,d)$	10.20	1.33	11.5	1.8	13.3
200	''101''	$1s$	$\leqslant 18(s,p,d)$	8.88	1.33	10.2	2.1	12.3
200	364[a]		$l=0-6$		0.0			14.9
200	20[b]			12.9				17.8
300	51[c]	$\leqslant 8(s,p)$	$\leqslant(12s,8p,3d)$	7.92			0.6	8.5
300	59	$1s$	$\leqslant 11(s,p,d)$	8.41	1.16	9.57	0.47	10.0
300	''101''	$1s$	$\leqslant 18(s,p,d)$	7.97	1.16	9.14	0.56	9.7
300	364[a]		$l=0-6$		0.1			10.8
300	20[b]			10.3				12.3
500	''101''	$1s$	$\leqslant 18(s,p,d)$	5.95	0.85	6.80	0.08	6.88
500	364[a]		$l=0-6$		0.06			7.08
500	20[d]			6.8				7.7
500	20[b]			7.2				7.8
625	''101''	$1s$	$\leqslant 18(s,p,d)$	5.08	0.72	5.80		5.8
700	''101''	$1s$	$\leqslant 18(s,p,d)$	4.66	0.66	5.32		5.3
700	20[b]			5.7				
750	51[c]	$\leqslant 8(s,p)$	$\leqslant(12s,8p,3d)$	4.66				4.68
750	''101''	$1s$	$\leqslant 18(s,p,d)$	4.42	0.62	5.04		5.0
1000	''101''	$1s$	$\leqslant 18(s,p,d)$	3.53	0.49	4.02		4.0
1000	20[d]			4.0				4.4
1000	20[b]			4.0				4.0
2000	''101''	$1s$	$\leqslant 18(s,p,d)$	2.00	0.25	2.25		

[a]Finite-Hilbert set of Hall *et al.* [8].
[b]Atomic plus probability-absorber states of Errea and Sánchez [4].
[c]Sturmian functions of Stodden *et al.* [1].
[d]Atomic plus R-space states of Henne *et al.* [3].

For the $3s$ initial state, only results with the single fully coupled basis, the largest 59-state basis $1s_{\mathrm{H}}$, $\leqslant 11(s,p,d)_{\mathrm{He}}$, have been compared with the Born results. Differences (not shown in Fig. 5) are large: a factor of 1.94, 2.09, 2.19, and 2.26 at energies 200, 500, 1000, and 2000 keV, respectively. On the other hand, for this same initial state with s,p coupling separate from d coupling, cross sections with the largest ''95-state'' basis, $1s_{\mathrm{H}}$, $\leqslant 17(s,p,d)_{\mathrm{He}}$, differ in Fig. 6(c) from the s,p,d-wave Born cross sections by +13%, 11%, 9%, and 9% at 200, 500, 1000, and 2000 keV, respectively. The ''95-state'' cross section is actually a sum of the cross sections using the separate bases $1s_{\mathrm{H}},\leqslant 17(s,p)_{\mathrm{He}}$ and $1s_{\mathrm{H}},\leqslant(\overline{3s},17d)_{\mathrm{He}}$, where the pseudostates $\leqslant\overline{3s}$ are those with the lowest three eigenvalues obtained using the limited basis $\leqslant 12s$. This basis is not very reliable for $\overline{3s}$. The pseudostate is significantly improved to $\overline{3s'}$ by enlarging the basis to $\leqslant 17s$. At the same time, the d basis has been slightly reduced, leading to a modified basis $1s_{\mathrm{H}},\leqslant(\overline{3s'},15d)_{\mathrm{He}}$ and a significantly improved composite basis of ''89 states'' $1s_{\mathrm{H}}$, $\leqslant(17(s,p),15d)_{\mathrm{He}}$. The ''89-state'' cross sections lie only 7%, 6%, 5%, and 5% above the s,p,d-wave Born cross sections at 200, 500, 1000, and 2000 keV, respectively. These differences are actually smaller than the differences from the s,p-wave Born cross sections of Sturmian cross sections without d states, but the same number of s and p states.

C. Comparison with other coupled-state results

1. Ground state

Shown in Table III are coupled-state cross sections for ionization in collisions between 200–2000 keV protons and $\mathrm{He}^+(1s)$ ions. For proton energies $E\leqslant 300$ keV, two sets of Sturmian results are presented since, as discussed in Sec. III B 2 (c), neither set is *a priori* judged superior: (1) The results of a 59-state calculation with the basis $1s_H$, $\leqslant 11(s,p,d)_{\mathrm{He}}$ and (2) the results obtained by separately using the bases $1s_H,\leqslant 18(s,p)_{\mathrm{He}}$ and $1s_{\mathrm{H}},(1s,\leqslant 18d)_{\mathrm{He}}$ to obtain a ''101-state'' result with the composite basis $1s_{\mathrm{H}}$, $\leqslant 18(s,p,d)_{\mathrm{He}}$. For $E\geqslant 500$ keV, the ''101-state'' basis is deemed better, and only results with it are shown. To make clearer the comparison with other coupled-state results, a contribution from neglected partial waves is extrapolated using the Born approximation as described in Sec. III A; these extrapolated results are also shown in Table III. Using the

TABLE IV. Coupled-state and Born-extrapolated cross sections (10^{-18} cm^2) for ionization and stripping in $p+\mathrm{He}^+(2s)$ collisions at various proton energies E.

				Ionization			Electron	Stripping
E (keV)	Number of functions	Proton center	Helium center	Coupled state	Born ext	Coupled state +Born	transfer	Coupled state +Born
200	59	1*s*	$\leqslant 11(s,p,d)$	36.3	28.8	65.1	0.9	66.0
200	''95''	1*s*	$\leqslant 17(s,p,d)$	35.9	28.8	64.7	0.9	65.6
200	364 [a]		$l=0-6$		4.5			59.4
300	59	1*s*	$\leqslant 11(s,p,d)$	27.2	19.4	46.6	0.2	46.8
300	''95''	1*s*	$\leqslant 17(s,p,d)$	27.1	19.4	46.5	0.2	46.7
300	364 [a]		$l=0-6$		3.1			41.5
500	59	1*s*	$\leqslant 11(s,p,d)$	18.3	11.7	30.0	0.0	30.0
500	''95''	1*s*	$\leqslant 17(s,p,d)$	18.3	11.7	30.0	0.0	30.0
500	364 [a]		$l=0-6$		1.9			26.5
625	59	1*s*	$\leqslant 11(s,p,d)$	15.3	9.3	24.6		
625	''95''	1s	$\leqslant 17(s,p,d)$	15.3	9.3	24.6		
1000	59	1*s*	$\leqslant 11(s,p,d)$	10.4	5.8	16.2		
1000	''95''	1*s*	$\leqslant 17(s,p,d)$	10.4	5.8	16.2		
2000	59	1*s*	$\leqslant 11(s,p,d)$	5.82	2.92	8.74		
2000	''95''	1*s*	$\leqslant 17(s,p,d)$	5.82	2.92	8.74		

[a]Finite-Hilbert set of Hall *et al.* [8].

Born approximation to include neglected partial waves is sometimes referred to as the Kummer transformation [38,39].

Also shown in the table are the 51-Sturmian-pseudostate results of Stodden *et al.* [1] using the 51-state basis $\leqslant 8(s,p)_{\mathrm{H}}, \leqslant (12s,8p,3d)_{\mathrm{He}}$. At 300 keV, the present unextrapolated ''101-state'' result lies within 0.6% of theirs, while at 750 keV the ''101-state'' result without and with a Born extrapolation for higher partial waves brackets the result of Stodden *et al.* by -5% and $+8\%$; the projectile-centered states in the 51-state basis should be of negligible importance at this high energy except to compensate for the deficiency of its target-centered part.

Also shown are the coupled-state results of Hall *et al.* [8] determined for $E=200$–500 keV (and lower energies) with a very large, single-center basis: the 364 states (counting contributing m sublevels) $\leqslant (13s,14p, \ldots ,19i)_{\mathrm{He}}$ (i.e., for each angular momentum $l \leqslant 6$, the basis label being the principal quantum number $n \geqslant l+1$ in our notation). The present coupled-state bases only include states with $l \leqslant 2$, and so have a more significant Born extrapolation for higher partial waves. On the other hand, since theirs is a single-center basis, Hall *et al.* could only determine the stripping (electron-removal) cross section; a small contribution from electron transfer at these energies is therefore added to the present results to compare with their stripping cross sections. It is seen that the stripping cross sections of Hall *et al.* are 12–21%, 8–11%, and 3% above the present results at $E=200$, 300, and 500 keV, respectively. At the lower energies, particularly 300 keV, the difference appears to exceed the estimated uncertainty in the present calculation. At 500 keV, the difference may possibly be explained by their tolerance in integrating equations over time, stated to be $\leqslant 3\%$ at these energies.

Also shown in Table III are results for both ionization and stripping extracted from the graphs of the results of two similar calculations: those of Henne *et al.* [3] and Errea and Sánchez [4], both obtained using a single-center basis of 10 He^+ states and 10 additional states which are intended to span the main part of the contributing space not included with the first 10 states. The additional states of Henne *et al.* are *R*-space states in a doorway approximation to the optical potential; those of Errea and Sánchez are other probability-absorber states or doorway states. The ionization cross sections of Henne *et al.* agree closely with the present Born-extrapolated coupled-state results at the overlapping energies of 500 and 1000 keV, while their stripping cross sections are about 10% above the present results at these energies. The ionization cross sections of Errea and Sánchez are 12–26%, 8–13%, and 6% above the present Born-extrapolated results at $E=200$, 300, and 500 keV, respectively; without the Born extrapolation in the present results, these differences would be larger. At these energies, the differences for stripping are larger than for ionization. [However, the graphically presented results of Errea and Sánchez for ionization, capture (not shown here), and stripping are numerically inconsistent at the lower energies.] At 700 and 1000 keV, the results agree within 2%. Not shown are the molecular-state results of Errea *et al.* [5] for ionization and stripping at the single overlapping energy of 200 keV; their result for ionization agrees with our extrapolated ''101-state'' result.

2. 2s state

Shown in Table IV are coupled-state cross sections for ionization in collisions between 200–2000 keV protons and

TABLE V. Coupled-state and Born-extrapolated cross sections (10^{-18} cm^2) for ionization in $p+\mathrm{He}^+(3s)$ collisions at various proton energies E. The results are obtained with an ''89-state'' $1s_{\mathrm{H}}$, $\leqslant(17(s,p),15d)_{\mathrm{He}}$ basis.

E (keV)	Coupled state	Born extrapolation	Coupled state + Born extrapolation
200	81	73	154
500	38	29	68
625	32	23	55
1000	21	15	36
2000	12	7	19

$\mathrm{He}^+(2s)$ ions. Unlike for the $1s$ initial state, results with the 59-state, fully coupled basis $1s_{\mathrm{H}},\leqslant 11(s,p,d)_{\mathrm{He}}$ agree very closely (to within at least 1%) with those using the composite basis, here the ''95-state'' basis $1s_{\mathrm{H}},\leqslant 17(s,p,d)_{\mathrm{He}}$ and, within the s,p,d manifold, both sets of results may be considered converged, as discussed in Sec. III B 2 (c). After estimating the significant contribution from higher partial waves and including a small contribution from electron transfer, these results may be compared with the only other available coupled-state results, those of Hall *et al.* [8] for $E=200$–500 keV (and lower energies). It is seen that their Born-extrapolated stripping cross sections lie 9–12 % below the present Born-extrapolated results at all energies. We cannot explain this discrepancy, particularly at $E=500$ keV, since our results appear to be converged for $l=0,1,2$ and since the Born approximation should be reliable for estimating the (significant) contribution from higher partial waves at this energy.

3. 3s state

Shown in Table V are coupled-state cross sections for ionization (and stripping) in collisions between 200–2000 keV protons and $\mathrm{He}^+(3s)$ ions. All reported coupled-state values are with the ''89-state'' composite basis, $1s_{\mathrm{H}}$, $\leqslant(17(s,p),15d)_{\mathrm{He}}$, described in Sec. III B 2 (c) and judged to be the most converged in view of the comparison with Born results at the higher energies. The present Born-extrapolated coupled-state results are estimated to be accurate to 5%. At the higher energies, the full Born results given in Sec. III A are probably still more reliable. Cross sections in Table V may also be considered to be stripping cross sections, since electron transfer has been shown to contribute negligibly ($<1\%$) at the tabulated energies. There do not appear to be any other coupled-state results for the $3s$ initial state.

D. Comparison with experimental results

At higher intermediate energies, experiments have generally measured total He^{2+} production (stripping) rather than ionization separated from the smaller electron-transfer component. Therefore, stripping rather than ionization cross sections are compared with experimental results in Fig. 7. Shown are the average of the best present coupled-Sturmian cross sections for p-$\mathrm{He}^+(1s,2s,3s)$ collisions along with the

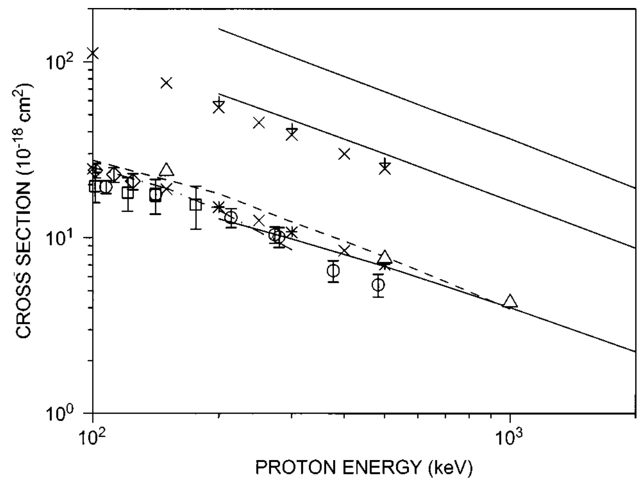

FIG. 7. Cross sections for stripping (electron removal) in collisions between protons and $\mathrm{He}^+(1s,\ 2s,$ or $3s)$ ions. The lower, middle, and upper results are for $1s$,$2s$, and $3s$, respectively. Coupled-state results: solid curve, average of the best present Sturmian results; dash-dotted curve, the largest-basis Sturmian results of Stodden *et al.* [1] ($1s$); crosses, plus signs, Hall *et al.* [8] ($1s$,$2s$), without and with Born extrapolation, respectively; dashed curve, Errea and Sánchez [4] ($1s$); triangles, Henne *et al.* [3] ($1s$). Experimental results ($1s$): diamonds, Rinn *et al.* [10]; squares, Watts *et al.* [9]; circles, Angel *et al.* [11].

coupled-state results of Hall *et al.* [8] (for $1s$,$2s$), Henne *et al.* [3], and Errea and Sánchez [4] (for $1s$). The experimental results of Watts *et al.* [9], Rinn *et al.* [10], and Angel *et al.* [11] for $1s$ are given with estimated total error limits (random plus systematic errors). To get a fuller picture, available results are shown down to 100 keV, although the present results are for $E\geqslant 200$ keV only; the $1s$ stripping cross section actually peaks at a somewhat lower energy than that shown, owing to the dominant contribution from electron transfer there. Also shown for completeness are the earlier Sturmian results of Stodden *et al.* [1] extending to lower energies using a larger projectile-centered basis but a smaller target-centered one. It is seen that up to 300 keV, the experimental results for stripping from the $1s$ state appear to favor the present results and those of Hall *et al*. over those of Henne *et al.* and Errea and Sánchez. Above 300 keV, all the theoretical results lie above the upper error limit of the experimental cross section.

IV. CONCLUSION

The first Born approximation is a benchmark for coupled-state ionization cross sections at higher energies. By gradually enlarging the coupled-Sturmian-pseudostate basis over a wide range and comparing the successive cross sections to the high-energy (Born) limit, their accuracy and, at higher intermediate energies, the extent to which the Born approximation fails, have been determined. Within the s,p,d target-centered manifold (augmented by a single projectile-centered state), coupled-Sturmian cross sections are estimated to be converged to 1% for the $1s$ and $2s$ initial states and 5% for the 3s initial state, except for 1s at proton energies $E \lesssim 300$ keV. Contributions from higher partial waves ($l \geqslant 2$) have been included by means of the Born approximation.

Disagreement with other existing coupled-state results for 1s and 2s is, for the most part, $\lesssim 10\%$. Where there is disagreement, the other coupled-state results lie above the present ones for 1s and below for 2s. Only for 1s at the lowest energies, 200 and 300 keV, is the relatively small discrepancy attributed at least in part to basis nonconvergence of the present calculation. However, the experimental results for 1s cannot distinguish the present results from those of Hall *et al.* at these two energies. There is a need for experimental results for the 1s state at higher energies $E \gtrsim 500$ keV, and for the 2s and 3s states at all energies.

ACKNOWLEDGMENTS

The authors thank James S. Cohen for suggesting the relevance of this calculation to a study of muon-catalyzed fusion and for several communications and discussions. Helpful discussions with Dmitry V. Fursa and Alisher S. Kadyrov on Sturmians are also acknowledged. Computations were performed on Pennsylvania State University's VM/ESA mainframe computer.

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