Triple-center treatment of electron transfer and ionization in He^{2+}-H and p-He^{+} collisions

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(Received 28 December 1987)

Cross sections have been calculated for electron transfer into the $2s$, $2p_0$, $2p_1$, and all states of He^+, and for ionization, in collisions between $^4He^{2+}$ ions and H($1s$) atoms. Cross sections have also been calculated for electron transfer into the ground state and all states of H, and for ionization, in collisions between protons and $^4He^+(1s)$ ions. The center-of-mass collision energies range from 1.6 to 40 keV. A coupled-state approach is taken using large triple-center bases of up to 34 states centered on the two nuclei and a third center chosen to be the equiforce point (saddle point of the potential) between the nuclei. The sensitivity of the cross sections to the size of basis is studied, and the ionization cross sections are found to be the more sensitive, particularly at lower energies. The electron-transfer cross sections in most cases are found to agree extremely well with larger-basis molecular-state results at generally lower energies and with double-center pseudostate results at higher energies, as well as with experimental results. The more sensitive ionization cross sections follow the trend of the experimental data, suggesting the considerable importance of saddle-point electrons as previously observed for p-H collisions.

I. INTRODUCTION

Electron transfer in collisions between He^{2+} ions and H($1s$) atoms is a basic, one-electron collision process, a prototype of resonant electron transfer in somewhat asymmetric systems. No less basic is electron transfer in collisions between protons and *ground-state* He^+ ions. In this very different process, the initial and primary final states are nonresonant and so the cross section is much smaller.

These two processes have been studied in detail with many coupled-molecular-state calculations.[1-12] Such calculations have necessarily been confined to lower-keV collision energies, at which the nuclear motion strongly couples only a few molecular states. [For He^{2+}-H($1s$) collisions, the primary states[1] are the initial state $2p\sigma$ and the electron-transfer states $2p\pi$, $3d\sigma$, and $2s\sigma$ degenerate with the initial state in the separated-atom limit; for p-$He^+(1s)$ collisions, the primary states[5] are the initial state $1s\sigma$ and the main electron-transfer state $2p\sigma$ as well as the state $2p\pi$ and $2s\sigma$, the latter three states being energetically quite far removed from the initial state.] With few exceptions for either collision system,[3-5,10,12] center-of-mass energies $E_{\text{c.m.}}$ have been kept to 4 keV or below. (The energy $E_{\text{c.m.}}$ is one-fifth of the energy E of the $^4He^{2+}$ or $^4He^+$ ion relative to a stationary H atom or proton.) At 4 keV the relative speed is only 0.45 a.u. At these low energies generally good agreement exists among the molecular-state and experimental[13-23] results.

Until recently (see the following),[12] only the ten-molecular-state calculations of Hatton, Lane, and Winter;[3] Winter and Hatton;[4] and Winter, Hatton, and Lane[5] with plane-wave translational factors extended to the somewhat higher energy $E_{\text{c.m.}} = 14$ keV. There, the calculations began to break down: In the case of He^{2+}-H($1s$) the $2s$ electron-transfer cross section is significantly below the experimental values;[13-15] for p-$He^+(1s)$ collisions, the electron-transfer cross section is 20–30 % below more reliable theoretical values.[24,25]

By higher energies such as this, an atomic-state basis is probably called for, or a large number of molecular states. There is an additional problem, particularly noticeable for the p-He^+ case: *Intermediate* coupling to ionization states significantly influences the small electron-transfer cross section.

Recently, Errea, Gómez-Llorente, Méndez, and Riera[12] have also reported higher-energy, molecular-state calculations with, however, norm-optimized translational factors. Their method minimizes couplings with neglected states and so can be extended to somewhat higher energies. However, the method cannot be extended too far into the "atomic-state energy range" due to the increasing importance of ionization states as open channels.

A general method is desirable which is accurately molecular in character at low energies and smoothly assumes a more atomic character as the energy is increased while also accounting for the continuum; the troublesome transitional energy region must be spanned. The triple-center method, developed by Anderson, Antal, and McElroy[26,27] and later extended by Lin, Winter, and Fritsch[28] and Winter and Lin[29,30]—all in the context of the very different, symmetric p-H($1s$) case—is such a method. By placing united-atom wave functions on a chosen third center between the two nuclei, as well as atomic wave functions on the nuclei themselves, the molecular character of the electronic wave function at low energies can be well represented; at higher energies, the atomic wave functions centered on the two nuclei may by themselves be adequate.

Anderson *et al.*[26] proposed that the third-center basis functions might, in addition, represent ionization, which gradually becomes more important as the collision energy is increased. Since they included only a single function on the third center, their basis is inadequate to represent

ionization. Winter and Lin[30] employed a much larger number of functions (16) on the third center, yielding an ionization cross section which approximately follows the energy dependence of (and is not far from) recent experimental results.[31] (The calculated electron-transfer cross sections[29] largely agree.)

The third-center functions allow for ionization—as well as its effect on electron transfer—in two main ways. First, as noted by Anderson *et al.*,[26] these functions, in the united-atom limit, have a large overlap with states of direct ionization and charge transfer to the continuum, centered on the target and projectile nuclei, respectively; to the extent that ionization occurs in close encounters, the third-center functions thus adequately represent these traditional mechanisms of ionization. Secondly, as pointed out by Winter and Lin,[30] a third mechanism should dominate at sufficiently low energies: ionization from the vicinity of the saddle point of the electron-nuclear potential, or equiforce point. At this point, the electron is pulled equally in both directions and thus avoids being trapped by either nucleus during the long time available in a slow collision. These saddle-point electrons in not-very-slow collisions have recently been "observed" by Olson, Gay, Berry, Hale, and Irby[32] in classical calculations and observed experimentally by Meckbach, Focke, Goñi, Suarez, Macek, and Menendez[33] and Olson *et al.*

Not having considered this additional possible mechanism for ionization, Anderson *et al.*[26] suggested that the center of nuclear charge be chosen as the third center. In the p-H($1s$) collision they treated, this point is identical to the equiforce point. In asymmetric collisions, such as He^{2+}-H or p-He^{+} collisions, on the other hand, the center of charge and equiforce points are distinct, the former being nearer the He nucleus, and the latter, nearer the proton. The choice of placement of the third center is thus an issue related to the saddle-point, "Wannier mechanism"[34] of ionization, which will be addressed in this paper by contrasting a limited test with the third center on the center of charge to the main results with center on the saddle point.

The plane-wave-factor, molecular-state approach of Bates and McCarroll[35]—applied by Hatton, Lane, and Winter;[3] Winter and Hatton;[4] and Winter, Hatton, and Lane[5]—is sometimes faulted (particularly at higher energies) for having unrealistic translational factors at small internuclear separations: The electronic molecular states unphysically travel with one nucleus or the other rather than being stationary with respect to the molecule as a whole. The triple-center approach eliminates—or at least reduces—this defect, since the third-center "molecular" states are stationary with respect to this center, which represents some average position of the two nuclei.

To treat ionization or its effect on electron transfer at the intermediate energies of interest here, double-center pseudostate approaches have almost exclusively been applied. In these approaches, a basis of approximate or exact bound atomic states on each nuclear center is augmented by pseudostates on one or both centers. Sturmian pseudostate, Callaway-Wooten pseudostate, and other pseudostate bases have been employed, respectively, by Winter;[24,36,37] Bransden, Noble, and Chandler;[38] and Fritsch and Lin[25,39] for the HeH^{+} collisional system. One of the Fristch-Lin bases—the so-called AO+ basis[25]—is closely related to the present triple-center basis: a double-center basis of bound atomic states is augmented by a small number of united-atom functions centered on the two nuclei rather than on the third center. Lüdde and Dreizler employed a double-center, Hylleraas basis without translational factors.[40] A large pseudostate basis was used by Reading, Ford, and Becker[41] with, however, only one function centered on the H nucleus; this so-called one-and-a-half-center basis is suitable at the higher intermediate energies where electron transfer may be treated as a perturbation.

The results of these double-center pseudostate as well as the molecular-state calculations will be compared in detail with the present triple-center results in Sec. III B. This comparison will be preceded in Sec. III A by a study of the sensitivity to the size of the triple-center basis. The method and computational details will be summarized in Sec. II. Atomic units are used except where indicated otherwise.

II. SUMMARY OF METHOD AND NUMERICAL TESTS

All triple-center calculations, and most of the others noted previously as well, have been carried out in the impact-parameter method assuming straight-line nuclear trajectories. The calculations of Refs. 2, 5, and 10 show that even at the lowest energy considered here ($E_{\text{c.m.}}=1.6$ keV), the resulting error in each electron-transfer cross section due to this choice of trajectory probably does not exceed 1% (except for the small p-He^{+} cross section for which the estimated error is 7%).

Following Anderson, Antal, and McElroy[26] and as applied by them and Winter and Lin[29,30] to p-H collisions, the time-dependent electronic wave function is expanded as a linear combination of traveling atomic orbitals on *three* centers,

$$\Psi(\mathbf{r},t)=\sum_{k,\alpha} a_{k\alpha}(\rho,t)\psi_{k\alpha}(\mathbf{r}_\alpha(\mathbf{r},t)) \times\exp(-iE_{k\alpha}t+iq_\alpha\mathbf{v}\cdot\mathbf{r}-\tfrac{1}{2}iq_\alpha^2v^2t)\ , \tag{1}$$

where α denotes the center A ($=H^{+}$), B ($=He^{2+}$), or C, and

$$q_\alpha=\begin{cases}-\frac{1}{2}, & \alpha=A\\ +\frac{1}{2}, & \alpha=B\\ p-\frac{1}{2}, & \alpha=C\ .\end{cases} \tag{2}$$

The $\psi_{k\alpha}$ and $E_{k\alpha}$ are atomic wave functions and energies of a hydrogenic atom of nuclear charge Z_α (where $Z_C=Z_A+Z_B$). In the above expression for q_α, the origin of coordinates has been assumed to be the midpoint of the internuclear line. However, following Bates,[42] the results are independent of the choice of origin.

For a finite basis, the results do, of course, depend on the choice of the third center C. In the case of proton-hydrogen collisions, this center was chosen by Winter and Lin[30] to be the equiforce point, which coincidentally

for that system is also the midpoint of the internuclear line and the center of charge, whereas Anderson *et al.*[26] and originally Winter and Lin[29] referred to the point as the center of charge. In the present heteronuclear case, these two points are distinct and C is here chosen to be the equiforce point rather than the center of charge. This is ensured by setting[30]

$$p=\frac{Z_A^{1/2}}{Z_A^{1/2}+Z_B^{1/2}}$$

in the definition of q_α, Eq. (2). This is the preferred choice on the physical grounds noted in the Introduction, and the results will confirm the suitability of this choice.

The expansion of the wave function, Eq. (1), is substituted into the time-dependent Schrödinger equation for the electron in the field of the nuclei A and B of fixed relative velocity $\mathbf{v}$ and impact parameter ρ. The resulting coupled, first-order differential equations are solved numerically[43] for the coefficients $a_{k\alpha}(\rho, t\rightarrow\infty)$ subject to the boundary conditions

$$a_{k\alpha}(\rho, t\rightarrow-\infty)=\delta_{k,1s}\delta_{\alpha\beta}\ ,$$

where $\beta=A$ or B is the nucleus to which the electron is initially bound. The method of solution has been described in detail in the triple-center paper of Winter and Lin[29] following an earlier paper of Winter[24] on double-center approaches.

Several numerical tests have been carried out at each projectile energy and one or more impact parameters (using bases of at least 18 states). These tests monitored the probabilities of electron transfer into the $1s$, $2s$, $2p_0$, and $2p_1$ states and ionization in He^{2+}-H($1s$) collisions. [For p-He^+($1s$) collisions, the probability of electron transfer into all states and of ionization was also monitored in some cases at one energy.]

Firstly, the coupled differential equations have been integrated using the chosen lower and upper truncation-error limits 10^{-6} and 10^{-4} (10^{-7} and 10^{-5} at lower energies) and then solved again using limits one-tenth as large. Absolute changes in the transition probabilities do not exceed 10^{-5}, and relative changes are at worst in the fourth digit.

Secondly, the internuclear separation beyond which coupling between states on different centers is neglected has been changed from the chosen value $64a_0$ to the value $(64\pm20)a_0$. The absolute changes in the transition probabilities are at most 6×10^{-5}, and the relative changes in almost all cases occur at worst in the fourth digit.[44]

Thirdly, the number of integration points in the two-dimensional integration over the prolate spheroidal coordinates λ and μ, used to calculate the two- and three-center charge-exchange matrix elements, was varied from the chosen values (16–32 λ points, 16–24 μ points). The resulting absolute changes do not exceed 5×10^{-4} and in almost all cases relative changes do not exceed one unit in the third digit.[45]

To obtain the individual $2s$,$2p_{0,1}$ transition probabilities, the coupled equations have been integrated to a chosen large value of z ($=vt$), $10\,000a_0$, in order to account for long-range coupling among the three states. A further extension to $z=100\,000a_0$ at one energy and impact parameter revealed changes in only the fifth digit.

As a further check of accuracy, probability has been found to sum to unity to within 2×10^{-5} in almost all production runs[46,47] except at higher energies where the transition probabilities are larger; there, the departure from unity does not exceed 7×10^{-5}.

The total cross sections are obtained from the calculated transition probabilities $P_{k\alpha}(\rho)=|a_{k\alpha}(\rho,\infty)|^2$ by integrating over impact parameters:

$$Q_{k\alpha}=2\pi\int_0^\infty P_{k\alpha}(\rho)\rho\,d\rho\ ,$$

evaluated using Simpson's rule, usually[48] to an accuracy of at least $\frac{1}{2}\%$.

III. RESULTS

Cross sections have been calculated for electron transfer and ionization in collisions between He^{2+} ions and H($1s$) atoms using several triple-center bases; see Table I. Corresponding cross sections for collisions between protons and $^4He^+$($1s$) ions have also been determined and are given in Table II. The center-of-mass energy $E_{c.m.}$ for which the results are reported ranges from 1.6 to 40 keV. (The cross sections for electron transfer into the *ground* state of He^+ in He^{2+}-H collisions are omitted from Table I, since by detailed balancing these are identical to the cross sections given in Table II for electron transfer into the ground state in p-He^+ collisions. At the lower He^{2+} energies $E\leq20$ keV, electron transfer into the ground state contributes negligibly to the total transfer cross section.)

A. Sensitivity to the size of basis

To simplify the study of the sensitivity to the size of basis, results have been calculated with four bases, each containing all states within specified principal quantum shells on the centers; couplings among all degenerate states (degenerate in the united- or separated-atoms limits) are potentially important when considered from the perspective of related molecular- and atomic-state approaches. The first and smallest basis consists of the following 15 states: the ground state of H, all states of He^+ with principal quantum number $n\leq2$, and all states on the third center with $n\leq3$. This basis should represent well the molecular states $1s\sigma$,$2s\sigma$, ..., $3d\delta$ (primarily[1,4,5] $1s\sigma$, $2s\sigma$, $2p\sigma$, $2p\pi$, $3d\sigma$, and $3d\pi$), since these states are included in both the united- and separated-atoms limits (with the exception of $3d\pi$ in the separated-atoms limit).

1. Role of excited states centered on the proton

The second basis consists of 18 states: the 15 states of the first basis plus the $n=2$ states centered on the proton. Referring to Table I, it is seen that in He^{2+}-H collisions the effect of these additional states on electron transfer into all states is small (at most 2%), except at the highest He^{2+} energy $E=200$ keV ($E_{c.m.}=40$ keV), where it is

TABLE I. Triple-center cross sections (in units of $Å^2$) for electron transfer into various states of He^+ and for ionization in collisions between $^4He^{2+}$ ions and H(1s) atoms. The collision energy with respect to the center-of-mass reference frame is $0.2E$, the energy E being that of the $^4He^{2+}$ ion relative to the H atom.

	Number of	Electron transfer					
E (keV)	states[a]	$2s$	$2p_0$	$2p_1$	2^b	All[c]	Ionization
8	15	1.3	2.6	2.0	5.9	5.9	0.35
8	18	1.29	2.54	2.01	5.84	5.84	0.189
8	24	1.32	2.65	2.09	6.06	6.33	0.023
20	15	2.11	5.18	3.81	11.1	11.1	0.987
20	18	2.16	5.08	3.79	11.0	11.0	0.611
20	24	2.17	5.16	3.84	11.2	11.7	0.133
70	15	1.86	5.24	3.70	10.8	10.9	1.42
70	18	1.92	5.20	3.47	10.6	10.7	1.25
70	24	2.02	5.08	3.41	10.5	11.7	0.90
70	34	2.15	5.11	3.24	10.5	11.8	1.10
125	15	1.28	3.05	1.39	5.72	5.94	4.41
125	18	1.18	2.98	1.50	5.66	5.88	3.13
125	24	1.04	2.80	1.75	5.59	7.44	2.12
125	34	0.96	2.66	1.81	5.43	7.06	2.96
200	15	0.577	0.828	0.326	1.73	1.92	6.56
200	18	0.608	0.931	0.321	1.86	2.05	4.76
200	24	0.601	0.975	0.380	1.96	3.11	4.20
200	34	0.608	1.03	0.446	2.08	3.34	4.62

[a]The 15 states $1s_A, 1s_B, 2s_B, 2p_{0,1B}, 1s_C, 2s_C, \ldots, 3d_{0,1,2C}$; the 18 states consist of the 15 states in addition to the $n=2$ states centered on A; the 24 states consist of the 18 states in addition to the $n=3$ states on B; and the 34 states consist of the 24 states in addition to the $n=4$ united-atom states on C, where A, B, and C denote the H nucleus, He nucleus, and equiforce point, respectively.
[b]Electron transfer into all $n=2$ states.
[c]Electron transfer into all *available* states.

TABLE II. Triple-center cross sections (in units of 0.1 $Å^2$) for electron transfer into the 1s state and all states of H and for ionization in collisions between protons and $^4He^+(1s)$ ions. The collision energy $E_{c.m.}$ is defined with respect to the center-of-mass reference frame.

	Number of	Electron transfer		
$E_{c.m.}$ (keV)	states[a]	1s	All[b]	Ionization
1.6	15	0.000 38		
1.6	18	0.000 381		
1.6	24	0.000 385		
4	15	0.0207	0.0207	0.001 00
4	18	0.0213	0.0216	0.000 76
4	24	0.0217	0.0220	0.000 28
14	15	0.852	0.852	0.174
14	18	0.851	0.896	0.136
14	24	0.869	0.899	0.0774
14	34	0.885	0.903	0.0652
25	15	2.22	2.22	0.508
25	18	2.25	2.39	0.360
25	24	2.27	2.33	0.344
25	34	2.19	2.24	0.496
25	33	2.24	2.32	0.393
40	15	1.86	1.86	1.73
40	18	1.93	2.28	1.33
40	24	2.20	2.54	0.785
40	34	2.35	2.67	0.697

[a]The 15, 18, 24, and 34 states as in footnote a of Table I; the 33 states consist of the 34 states in addition to $5s_C, 5p_{0,1C}$ and without $4f_{0,1,2,3C}$.
[b]Electron transfer into all *available* states.

7%. Electron transfer is predominantly[1] into the states $2s$, $2p_0$, and $2p_1$ of He^+; even for these individual states, the effect of the excited states of H is seen to be less than 8% (except for a 12% effect at the highest energy for $2p_0$).

Referring to Table II, it is seen that for p-He^+ electron transfer into the ground state of H, the effect of excited H states is also small, less than 3% (except for a 4% effect at the highest energy $E_{c.m.}=40$ keV). On the other hand, for p-He^+ electron transfer into *all* states of H, this effect increases from 4% to 23% as the energy $E_{c.m.}$ increases from 4 to 40 keV. Thus electron transfer directly to the excited states of H becomes increasingly important, as is well known,[24] while indirect coupling of these states to the ground state of H is unimportant.

The $n=2$ states of H significantly affect ionization in both He^{2+}-H and p-He^+ collisions; in each case, the cross sections are *lowered* by an average of about 25% for energies $E_{c.m.}=4$–40 keV. The effect is not strongly energy dependent over this energy range. However, tests for He^{2+}-H collisions show that the effect becomes large (a factor of 2) at the lowest energy $E_{c.m.}=1.6$ keV, reflecting the increasing difficulty of representing the very small ionization channels as the energy is decreased. (The negligibly small p-He^+ ionization cross section at low energies would be expected to be even more sensitive.)

2. *Role of excited states centered on the He nucleus*

The third basis consists of 24 states: the 18 states of the second basis plus the $n=3$ atomic states centered on the helium nucleus. Referring to Table II, it is seen that for electron transfer into the ground state (or all states) of H in p-He^+ collisions, the effect of these He-centered states is negligible, at most 2%, except at the highest energy $E_{c.m.}=40$ keV, where it is about 10%.

For electron transfer into all states of He^+ during He^{2+}-H collisions, the effect is small but not insignificant (6–9%) at the lower energies $E_{c.m.}=1.6$–14 keV (see Table I). As the energy is increased, the effect grows significantly (to 50% by $E_{c.m.}=40$ keV), primarily reflecting electron transfer directly into these states rather than indirect coupling to the $n=2$ states of He^+. The importance of electron transfer into excited states of He^+ with $n\geq 3$ has been previously pointed out by Bransden and Noble.[49]

Referring to Tables I and II, these additional He^+ states are seen to decrease the cross sections for ionization in He^{2+}-H and p-He^+ collisions by up to 40% at energies $E_{c.m.}=14$–40 keV; the effect is even larger at lower energies. Without these He^+ states, flux apparently becomes trapped on the third center, overestimating ionization.

3. *Role of "excited states" centered on the third center*

The fourth and largest basis consists of 34 states: the 24 states of the third basis plus all the $n=4$ states on the chosen third center, the equiforce point. These states are the $n=4$ atomic states in the united-atom limit. Referring to Tables I and II, it is seen that their effect on electron transfer into all states is small, both for He^{2+}-H and p-He^+ collisions: at most 2% for $E_{c.m.}\leq 14$ keV. (The effect for He^{2+}-H collisions at the lower energy $E_{c.m.}=4$ keV is estimated from results at only two to three impact parameters, noted in Sec. III B.) Even at the highest energy $E_{c.m.}=40$ keV the effect does not exceed 7%.

The effect on individual-state ($2s$, $2p_0$, and $2p_1$), He^{2+}-H cross sections is only somewhat larger: up to 7% for energies $E_{c.m.}\leq 14$ keV. At the highest energy the effect is fairly large (17%) only for the $2p_1$ state.

On the other hand, the effect on ionization in both He^{2+}-H and p-He^+ collisions is quite large: up to about 40% for energies $E_{c.m.}\geq 14$ keV (and still larger at lower energies in the tested case of He^{2+}-H collisions).

In view of this large effect, an additional calculation was carried out for p-He^+ collisions at one of the higher energies ($E_{c.m.}=25$ keV): the states $5s_C$,$5p_{0,1C}$ were added while the states $4f_{0,1,2,3C}$ were removed (to limit the already large computing time[50]), yielding a 33-state basis. Referring to Table II, it is seen that this lowers the ionization cross section by 21%, whereas the previously added $n=4$ states raise it by 44%; thus some sort of convergence may be setting in. [The effect of these $n=5$ states (and the removed $4f$ states) on the p-He^+ electron-transfer cross section is seen to be small: at most 4%.]

Finally, a limited test of the sensitivity to placement of the third center was carried out at one energy ($E_{c.m.}=4$ keV) and impact parameter ($\rho=0.7a_0$). [The tests were performed for He^{2+}-H($1s$) collisions; by detailed balancing the cross section for electron transfer to the ground state equals that for transfer to the ground state in p-He^+($1s$) collisions.] The center was chosen to be the center of charge (nearer the He nucleus) rather than the equiforce point (nearer the proton). In an 18-state calculation, the probability of transfer to the ground state is 15% lower than the corresponding value obtained with the third center on the equiforce point, while the probability of ionization is almost a factor of 2 higher. These center-of-charge results are also farther from other theoretical results (to be presented in Sec. III B) than are the equiforce-point results; the latter will be seen to be extraordinarily close in the case of electron transfer. The placement of the third center at the center of charge (close to the He nucleus) apparently carries too much flux away from the He nucleus and onto the third center.

B. Comparison with other theoretical results

1. *Electron transfer into all states in He^{2+}-H collisions*

Coupled-state cross sections for electron transfer into all states of He^+ in He^{2+}-H collisions are given in Table III. Of the molecular-state results, only the plane-wave-factor results of Hatton, Lane, and Winter[3] and Winter and Hatton[4] have been reported up to the He^{2+} energy $E=70$ keV. (The recent, norm-optimized translational-factor results of Errea, Gómez-Llorente, Méndez, and Riera[12] extend to $E=64$ keV.) The present triple-center results are in extraordinarily good agreement (within 4%) with these plane-wave-factor results, even at this higher energy. The agreement with the optimized-trans-

TABLE III. Coupled-state cross sections (in units of $Å^2$) for electron transfer into all states of He^+ in He^{2+}-H collisions at various He^{2+} energies E (keV) using triple-center, double-center, and molecular bases.

Type of basis	Number of functions	Authors	E (keV) 8	20	70	200
Molecular with plane-wave factors	10	Hatton, Lane, and Winter	6.30	12.2	12.1	
Molecular with optimized translational factors	10	Kimura and Thorson	6.15	11.23		
Molecular with optimized translational factors	5	Crothers and Todd	5.9[a]	13[a]		
Molecular with common translational factor	10	Vaaben and Taulbjerg	5.19	9.63		
Molecular with Vaaben-Taulbjerg factor	4	van Hemert, van Dishoeck, van der Hart, and Koike	4.76	9.58		
Molecular with norm-optimized factors	10	Errea, Gómez-Llorente, Méndez, and Riera	6.19	11.98		
Double-center atomic	20	Bransden, Noble, and Chandler		10.5[a]	12[a]	3.6[a]
Double-center Hylleraas	Mixed[b]	Lüdde and Dreizler	6.47	10.9		2.95
Double-center Sturmian	19–24	Winter		11.1	11.0	3.74
Triple-center atomic	24 or 35[c]	Winter (this work)	6.33	11.7	11.8	3.34

[a]Graphical or interpolated values.
[b]Different numbers of functions are used at different internuclear separations.
[c]The 24 or 34 states defined in footnote a of Table I.

lational-factor results of Kimura and Thorson[7] and of Errea *et al.*[12] is equally outstanding up to the maximum common energy of the results, $E=20$ keV. These three molecular-state calculations all employ ten states which, however, are different; the different states and different translational factors are evidently unimportant here. On the other hand, the five-molecular-state results of Crothers and Todd[8] differ by 11% from the present results.

At higher energies, a double-center atomic-state or modified atomic-state (e.g., Sturmian) approach is probably to be preferred over the molecular-state approaches. It is seen in Table III that the triple-center atomic-state and double-center Sturmian[24] results agree to within 7%, except at the highest energy ($E=200$ keV), where the triple-center value is lower by 11%. There, it is also lower than the previously noted double-center, purely atomic-state result.[38] This difference in part results from the neglect of excited states of He^+ with $n \geq 4$ in the present triple-center calculation.

A more detailed comparison is of the impact-parameter dependences $\rho P(\rho)$ versus ρ shown in Figs. 1–4 for the triple-center atomic, plane-wave-factor molecular,[3,4] and double-center Sturmian[24] approaches. Particularly in the comparison of the triple-center and plane-wave-factor molecular results, the agreement persists to this level of detail. Also shown in Fig. 2 is the recent, norm-optimized translational-factor curve of Errea *et al.*[12] at the He^{2+} energy $E=20$ keV. The present results are generally even closer to this curve than to the others. At the highest energy ($E=200$ keV), the triple-center curve is seen to be uniformly below the Sturmian curve over a wide range of impact parameters, leading to the somewhat lower integrated cross section noted in the preceding paragraph.

2. *State-selective electron transfer in He^{2+}-H collisions*

Coupled-state cross sections for electron transfer into the individual states $2s$, $2p_0$, and $2p_1$ during He^{2+}-H collisions are given in Table IV. A comparison of these cross sections provides a more sensitive test than that for transfer into all states noted in Sec. III B 1.

It is seen that at energies $E \leq 20$ keV, triple-center and plane-wave-factor, molecular-state results[3,4] for each state agree fairly closely (within 9%), albeit not as well as noted previously for electron transfer to all states. In this energy range, there is comparable agreement (within 11%) with the optimized translational-factor, molecular-state results of Kimura and Thorson.[7] The recent, norm-optimized translational-factor, molecular-state results of Errea *et al.*,[12] reported at the overlapping energies 8 and 20 keV, agree very well with the triple-center results for the $2s$ state and the combined $2p$ state reported (all within 7%), although, again, not as well as does the summed cross section. The agreement (within 30%) with the five-state, Crothers-Todd result[8] is also not as good as

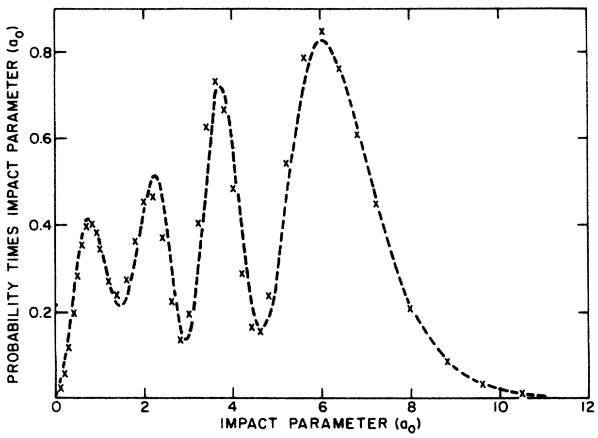

FIG. 1. Probability times impact parameter for electron transfer into all states of He^+ during collisions of 8-keV (laboratory energy) $^4He^{2+}$ ions with H(1s) atoms. Dashed curve, 10-molecular state with plane-wave translational factors (Refs. 3 and 4); crosses, 24 triple center (this work).

for the summed cross section. The limited-basis, molecular-state results of van Hemert, van Dishoeck, van der Hart, and Koike,[10] using the Vaaben-Taulbjerg[6] translational factor, differ from the present results at these energies by an average of about 20%, both for electron transfer into individual states and for electron transfer into all states.

Of all the molecular-state results, only plane-wave-factor results have been reported at the higher energy

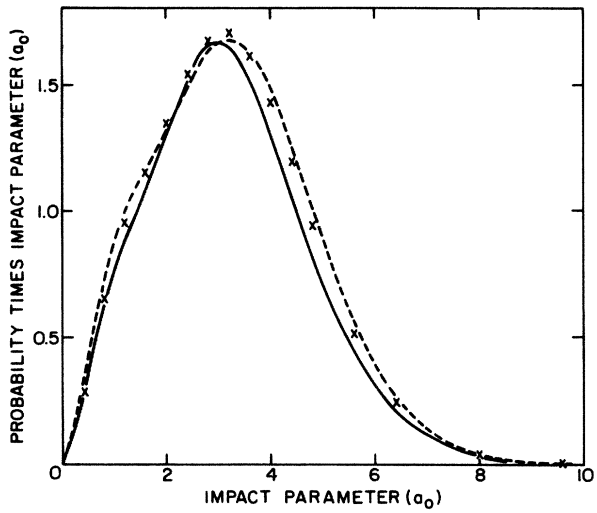

FIG. 3. Probability times impact parameter for 70-keV $^4He^{2+}$-H collisions. The results are labeled as in Fig. 1, with the addition that the solid curve is a 19-Sturmian pseudostate result (Ref. 24) and the exception that the triple-center results are 34-state results (this work).

$E=70$ keV. It is seen that at this energy there is significant disagreement with the triple-center results: the 2s cross section using the molecular-state approach is about a factor of 2 too low, probably reflecting the inadequate basis size (ten states) or translational factors at this energy. (See also the comparison with experimental results to follow.)

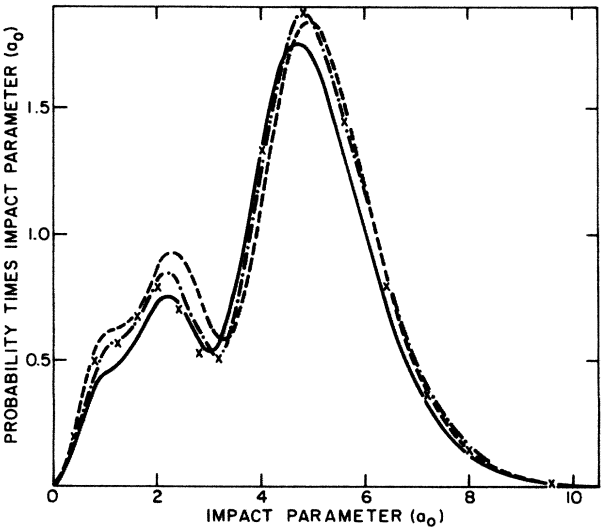

FIG. 2. Probability times impact parameter for 20-keV $^4He^{2+}$-H collisions. The results are labeled as in Fig. 1, with the following additions: solid curve, 21 Sturmian pseudostate (Ref. 24); dot-dashed curve, 10-molecular state with norm-optimized translational factors (Ref. 12). Not shown are 36-state triple-center values at the impact parameters $0.8a_0$, $2.0a_0$, and $4.8a_0$, which differ, respectively, by 1.6%, -1.9%, and 0.4% from the corresponding 24-state values.

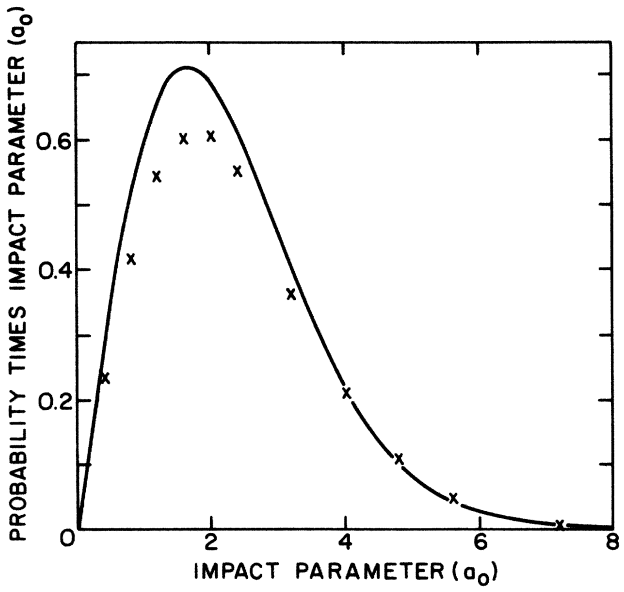

FIG. 4. Probability times impact parameter for 200-keV $^4He^{2+}$-H collisions. The results are labeled as in Fig. 1, with the addition that the solid curve is a 24-Sturmian pseudostate result (Ref. 24) and the exception that the triple-center results are 34-state results (this work).

TABLE IV. Coupled-state cross sections (in units of $Å^2$) for electron transfer into the $2s$, $2p_0$, and $2p_1$ states of He^+ in He^{2+}-H collisions at various He^{2+} energies E using triple-center, double-center, and molecular bases.

			E (keV)							
			8			20			70[a]	200
Type of basis	Number of functions	Authors	$2s$	$2p_0$	$2p_1$	$2s$	$2p_0$	$2p_1$	$2s$	$2s$
Molecular with plane-wave factors	10	Hatton, Lane, and Winter ($2s$) and Winter and Hatton	1.27	2.59	2.10	2.37	4.88	4.14	1.15	
Molecular with optimized translational factors	10	Kimura and Thorson	1.21	2.65	2.02	2.18	4.66	3.70		
Molecular with optimized translational factors	5	Crothers and Todd	1.46			2.90				
Molecular with Vaaben-Taulbjerg factor	4	van Hemert, van Dishoeck, van der Hart, and Koike	1.20	2.04	1.52	2.25	4.03	3.30		
Molecular with norm-optimized factors	10	Errea, Gómez-Llorente, Méndez, and Riera	1.24			2.20				
Double-center atomic	20	Bransden, Noble, and Chandler				2.3[b]			1.7[b]	0.4[b]
Double-center Hylleraas	Mixed[c]	Lüdde and Dreizler	1.76			2.51				0.26
Triple-center atomic	24 or 34[d]	Winter (this work)	1.32	2.65	2.09	2.17	5.16	3.84	2.15	0.608

[a]At 70 keV, the plane-wave factor, molecular-state values of Winter and Hatton for the $2p_0$ and $2p_1$ states are, respectively, 4.92 and 4.16 $Å^2$.
[b]See footnote a, Table III.
[c]See footnote b, Table III.
[d]See footnote c, Table III.

Consider now the double-center, 20-atomic-state results of Bransden, Noble, and Chandler.[38] Their result for $2s$ is seen to agree well (within 10%) with the present triple-center result at the energy $E=20$ keV, but at higher energies it departs significantly, perhaps reflecting the need to represent the ionization channels which they omitted.

The double-center, Hylleraas-basis results of Lüdde and Dreizler,[40] which agree well for electron transfer into all states, do not agree very well for transfer into the $2s$ state, particularly at higher energies; this may be due to the omission of translational factors in their basis.

3. *Electron transfer in p-He$^+$ collisions*

Coupled-state cross sections for electron transfer into the ground state and into all states of H in p-He$^+$ collisions are given in Table V. Consider only the dominant process of electron transfer into the ground state; at lower energies, the corresponding comparison for transfer into all states is almost identical, whereas at higher energies, where excited states begin to contribute, the cross sections are a little more sensitive to the method used.

Other than the present results (and one-and-a-half-center results[41]), the largest basis results are the double-center, Sturmian pseudostate results.[24,36,37] [A basis of 35 functions was used except at the lowest energy of these calculations ($E_{\text{c.m.}}=4$ keV), where 21 functions were used.] It is seen that there is extremely good agreement with these results (within 3%) over the full overlapping range of energies $E_{\text{c.m.}}=4$–40 keV. Both the Sturmian and triple-center methods to some extent account for intermediate coupling to ionization states and for molecular effects, so agreement is perhaps to be expected. The double-center pseudostate (AO +) calculation of Fritsch and Lin[25] is closely related to the present triple-center calculation. Their calculation employs all separated-atoms states up to $n=2$ on the appropriate centers and, in addition, united-atom states up to $n=2$ on both centers—16 functions in all. The present calculation also includes $n=3$ separated-atoms states on the He center and united-atom functions up to $n=3$ or 4 (but on the third center). At the previously-noted energies ($E_{\text{c.m.}}=4$–40 keV) there is good agreement with their graphical values (within 9%). A comparison with their results at the single lower energy ($E_{\text{c.m.}}=1.6$ keV) will be made in the following.

Consider now the molecular-state results: the plane-wave-factor results of Winter, Hatton, and Lane,[5] the optimized translational-factor results of Kimura and Thorson,[7] and the recent norm-optimized translational-factor results of Errea, Gómez-Llorente, Méndez, and Riera.[12] At the "higher molecular-state energy" $E_{\text{c.m.}}=4$ keV, there is seen to be very good agreement of the present results (within 5%) with the results of Winter *et al.* and fairly good agreement (within 11%) with the results of Kimura and Thorson. At the higher energy $E_{\text{c.m.}}=14$ keV, the plane-wave-factor, molecular-state result is at least 20% too low, which has been attributed by Winter[24] and Fritsch and Lin[25] to the failure of the molecular-state calculations to account for the increasingly important intermediate coupling to the continuum as the energy is increased; this coupling is unimportant to the much larger cross section at this energy for electron transfer into all states of He$^+$ during He^{2+}-H collisions. The recent calculation with norm-optimized translational factors, noted above,[12] minimizes this coupling to the continuum (and other neglected states). The agreement with the results of this calculation is extraordinarily good (within 3%) over the wide range of energies $E_{\text{c.m.}}=4$–40 keV.

Consider now the lowest-energy ($E_{\text{c.m.}}=1.6$ keV) triple-center cross section. This cross section is 18%, 25%, and 31% above the other coupled-state values noted in Table V [respectively, the molecular-state result of Winter, Hatton, and Lane;[5] the double-center pseudostate (AO +) result of Fritsch and Lin;[25] and the molecular-state result of Kimura and Thorson[7]]. The origin of this discrepancy among the four cross sections is discussed later, when the impact-parameter dependence is presented.

At higher energies, two sets of double-center, 23-pseudostate results have been reported by Bransden, Noble, and Chandler.[38] Both basis sets include atomic states up to $n=2$ on each center and an additional set of Callaway-Wooten pseudostates on the H nucleus for basis A and on the He nucleus for basis B. Only the results of basis A are given in Table V. Both bases yield results below the present triple-center results, the results with basis A being at most 10% below the present results.

To test the triple-center approach further, probability times impact parameter $\rho P(\rho)$ is plotted in Figs. 5–8 versus impact parameter ρ at energies $E_{\text{c.m.}}=1.6$, 4, 14, and 40 keV against some other coupled-state results, including the double-center Sturmian[24,36,37] and plane-wave-factor, molecular-state[5] results. The extraordinarily good agreement with the integrated Sturmian results, noted previously, is seen to extend to the impact-parameter dependence as well, over the full overlapping energy-range $E_{\text{c.m.}}=4$–40 keV. Not shown in Fig. 6 is the double-center, 16-pseudostate (AO +) curve of Fritsch and Lin[25] at $E_{\text{c.m.}}=14$ keV; this curve also agrees well with the triple-center results. At this energy the plane-wave-factor, molecular-state curve is significantly too low at the important impact parameters; this leads to the integrated cross section also being too small, as noted previously. On the other hand, the recent, molecular-state curve of Errea *et al.*[12] using norm-optimized translational factors is seen to agree closely with the present triple-center results, although not quite as well as does the Sturmian curve. At the highest energy ($E_{\text{c.m.}}=40$ keV) the norm-optimized translational-factor approach gives the same integrated cross section as the triple-center approach (to $\frac{1}{2}$%); however, compared to both the triple-center and Sturmian results, the $\rho P(\rho)$ curve with this method (not shown) peaks at significantly larger values of ρ.

Shown in Fig. 5 is the graph of $\rho P(\rho)$ versus ρ at the lowest energy $E_{\text{c.m.}}=1.6$ keV. The triple-center points closely follow the shape of the molecular curve, but are 15–20 % higher at impact parameters which contribute

TABLE V. Coupled-state cross sections (in units of 0.1 Å^2) for electron transfer into the ground state and into all states of H in p-^{4}He$^+$($1s$) collisions at various center-of-mass energies $E_{c.m.}$ using triple-center, double-center, and molecular bases.

Type of basis	Number of functions	Authors	State(s)[a]	$E_{c.m.}$ (keV) 1.6	4	14	25	40
Molecular with plane-wave factors	10	Winter, Hatton, and Lane	$1s$=all	0.000 323	0.0228	0.716		
Molecular with optimized translational factors	10	Kimura and Thorson	$1s$	0.000 282	0.0194			
			all	0.000 284	0.0199			
Molecular with norm-optimized factors	10	Errea, Gómez-Llorente, Méndez, and Riera	$1s$		0.022	0.861		2.34
			all		0.023	0.927		2.80
Double-center pseudostate (basis A)	23	Bransden, Noble, and Chandler	$1s$				2.0[b]	2.3[b]
			all				2.1[b]	2.5[b]
Double-center psuedostate	16	Fritsch and Lin	$1s$	0.000 30[b]	0.023[b]	0.95[b]	2.0[b]	2.2[b]
Double-center Hylleraas	Mixed[c]	Lüdde and Dreizler	$1s$	0.004	0.07			2.1
Double-center Sturmian	21[d] or 35	Winter	$1s$		0.0211	0.911	2.14	2.30
			all			0.964	2.36	2.72
Triple-center atomic	24 or 34[e]	Winter (this work)	$1s$	0.000 385	0.0217	0.885	2.19	2.35
			all		0.0220	0.903	2.24	2.67

[a]Cross sections marked "all" are for electron transfer into all *available* states.
[b]See footnote a, Table III.
[c]See footnote b, Table III.
[d]This smaller Sturmian basis is used at 4 keV only.
[e]See footnote c, Table III.

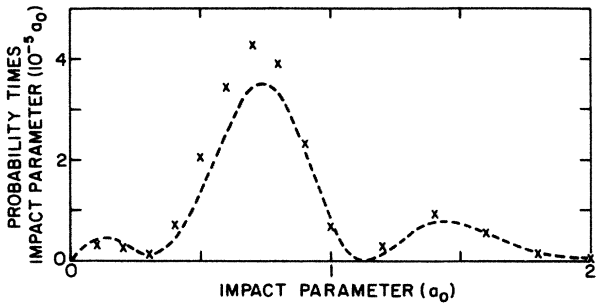

FIG. 5. Probability times impact parameter for electron transfer into the ground state of H in 1.6-keV (c.m.) p-$^4He^+$ collisions. Dashed curve, 10-molecular state with plane-wave translational factors (Ref. 5); crosses, 24 triple center (this work).

most significantly to the integrated cross section. The triple-center points also lie above the double-center pseudostate (AO +) curve (not shown) by about the same amount. This discrepancy is largely due to the smaller, less converged basis used in calculations other than the present triple-center ones. To illustrate this, the six states $3s_C$, $3p_{0,1C}$, $3d_{0,1,2C}$ have been removed from the smallest triple-center basis (the 15-state basis) to form a basis of the nine states $1s_A$, $1s_B$, $2s_B$, $2p_{0,1B}$, $1s_C$, $2s_C$, $2p_{0,1C}$. This basis is identical to the 16-state basis of Fritsch and Lin, except that the united-atom states $1s_C$, $2s_C$, $2p_{0,1C}$ are placed on the third center rather than on the nuclei A and B and except that the states $2s_A$, $2p_{0,1A}$ are omitted. [The omitted states on $A(=H^+)$ have previously been shown to have a negligible ($<2\%$) effect.] The result of a calculation at one impact parameter with this nine-state, triple-center basis agrees closely (within a few percent) with the 16-state, AO + value. At this low energy the very small electron-transfer probability is sensitive to the inclusion of the $n=3$ united-atom states (probably mainly $3d_0$) and other states, despite their being energetically removed from the lower-lying states; see also Ref. 5. Different translational factors may also play a role.

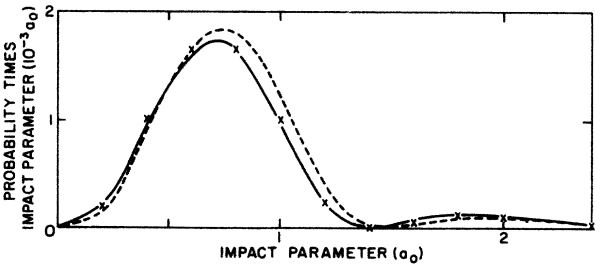

FIG. 6. Probability times impact parameter for 4-keV p-$^4He^+$ collisions. The results are labeled as in Fig. 5, with the additions labeled as in Fig. 2. Not shown are 36-state triple-center results at the impact parameters $0.8a_0$ and $1.8a_0$, which differ, respectively, by $+0.000\,02a_0$ and $-0.000\,02a_0$ from the corresponding 24-state values shown.

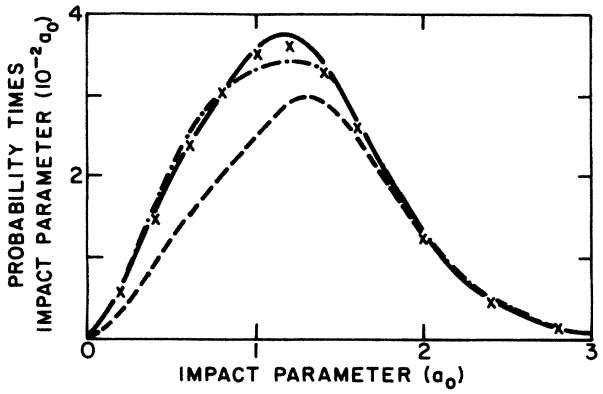

FIG. 7. Probability times impact parameter for 14-keV p-$^4He^+$ collisions. Dashed curve, 10-molecular state with plane-wave translational factors (Ref. 5); dot-dashed curve, 10-molecular state with norm-optimized translational factors (Ref. 12); solid curve, 35 Sturmian pseudostate (Ref. 36); crosses, 34 triple center (this work).

4. *Ionization in p-He$^+$(1s) collisions*

Other than the present cross sections there do not appear to be any coupled-state results for ionization in He^{2+}-H collisions. For ionization in p-He^+ collisions there are two sets of double-center pseudostate results at the higher energies $E_{c.m.} \geq 25$ keV: the Sturmian results of Winter[36,37] and the results of Fritsch and Lin;[39] see Table VI. The triple-center cross section is a factor of 2–3 above the double-center values at the energy $E_{c.m.} = 25$ keV, while at 40 keV the difference is reduced to 30–50%. These differences are similar to those between double- and triple-center results for p-H collisions at comparable energies.[30] The differences probably exceed the sensitivity to the size of the triple-center atomic-state basis estimated in Sec. III A and may reflect

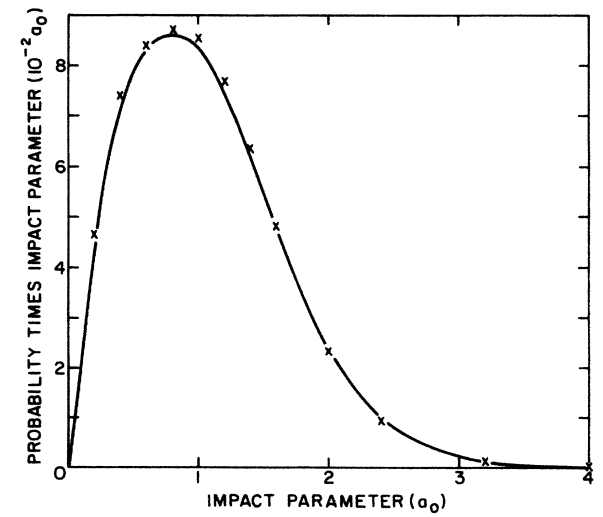

FIG. 8. Probability times impact parameter in 40-keV p-$^4He^+$ collisions. The curves are labeled as in Fig. 7.

TABLE VI. Coupled-state cross sections (in units of 0.1 Å^2) for ionization in p-^{4}He$^+$($1s$) collisions at two center-of-mass energies $E_{c.m.}$ using triple-center atomic and double-center pseudostate bases.

Type of basis	Number of functions	Authors	$E_{c.m.}$ (keV) 25	40
Double-center pseudostate	20–23	Fritsch and Lin	0.179	0.50[a]
Double-center Sturmian pseudostate	35	Winter	0.136	0.399
Triple-center atomic	33 or 34	Winter (this work)	0.393	0.697

[a]Graphically interpolated values.

the importance of saddle-point electrons, which are better accounted for in the triple-center approach. Bransden[51] has recently emphasized that accurate ionization cross sections are more difficult to calculate at these intermediate energies than are electron-transfer cross sections.

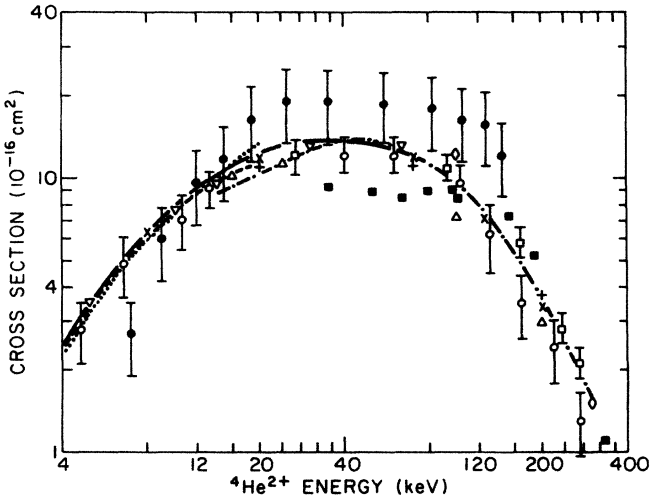

FIG. 9. Cross sections for electron transfer into all states of He^+ in $^4He^{2+}$-H collisions. Theoretical results: ×, the present 24- to 34-state triple-center results; +, the 19- to 24-Sturmian pseudostate results (Ref. 24); ——, the 10-molecular-state results with plane-wave factors of Hatton, Winter, and Lane (Refs. 3 and 4); — — —, the 10-molecular-state results of Kimura and Thorson with optimized translational factors (Ref. 7); ▽, the 10-molecular-state results of Errea *et al.* with norm-optimized translational factors (Ref. 12); · · · ·, the 5-molecular-state results of Crothers and Todd with optimized translational factors (Ref. 8); —·—·—·, the 20-atomic-state results of Bransden *et al.* (Ref. 38); △, the double-center Hylleraas results of Lüdde and Dreizler (Ref. 40); ◇, the one-and-a-half-center results of Reading *et al.* (Ref. 41); ■, the classical results of Olson *et al.* (Ref. 16). The experimental results: ○, Shah and Gilbody (Ref. 13) and Nutt *et al.* (Ref. 14); ●, Bayfield and Khayrallah (Ref. 15); □, Olson *et al.* (Ref. 16). Some data are for $^3He^{2+}$ projectiles at equivalent velocities. For clarity some overlapping values are omitted.

C. Comparison with experimental results

The experimental and theoretical results for electron transfer into all states of He^+ in He^{2+}-H($1s$) collisions are shown in Fig. 9. The experimental results of Shah and Gilbody[13] (and Nutt, McCullough, Brady, Shah, and Gilbody[14] at the lowest energies) and of Bayfield and Khayrallah[15] include both estimated random and systematic errors. The triple-center results are in excellent agreement with the data of Shah and Gilbody and Olson, Salop, Phaneuf, and Meyer[16] at all energies.

Shown in Figs. 10 and 11, respectively, are the results for electron transfer into the $2s$ and $2p$ states in He^{2+}-H($1s$) collisions. For electron transfer into the $2s$ state, the triple-center results agree well with most of the experimental results except at the He^{2+} energy $E=20$ keV, where the triple-center result is above the upper total ex-

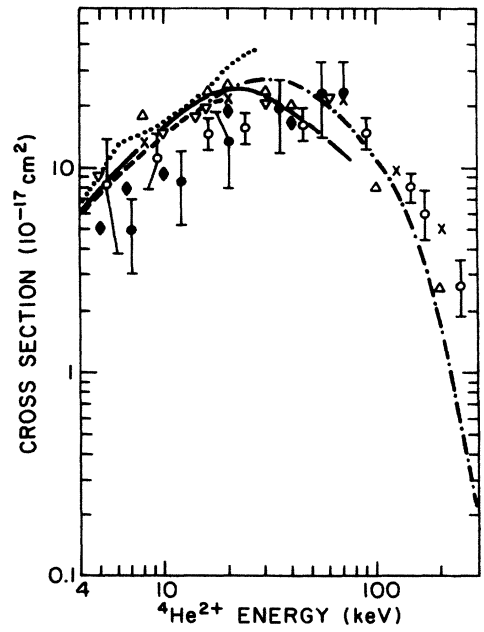

FIG. 10. Cross sections for electron transfer into the $2s$ state of He^+ in He^{2+}-H collisions. The notation is as in Fig. 9, with the following additional experimental data: ♦, Ćirić *et al.* (Ref. 17).

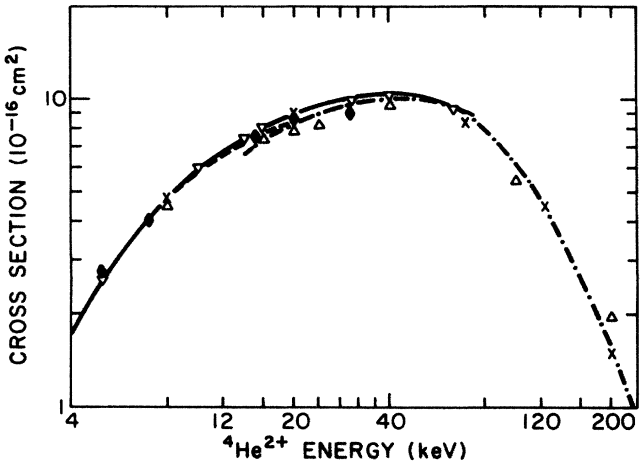

FIG. 11. Cross sections for electron transfer into the $2p$ state of He^+ in $^4He^{2+}$-H collisions. The notation is as in Fig. 9, with the following additional experimental data: ♦, Ćirić *et al.* (Ref. 18).

perimental error limit by about 15%. At 70 keV the experimental data agree with the present triple-center result rather than the ten-molecular-state result.[3,4] For electron transfer into the $2p$ state, it is seen in Fig. 11 that there is excellent agreement between the present triple-center results and the experimental results of Ćirić, Dijkkamp, Vlieg, and de Heer[18] available at the lower energies. (Experimental error bars are not given by Ćirić *et al.*) To test the theoretical approaches further, it would be desirable to have experimental $2p$ cross sections at higher energies also, as well as individual $2p_0$ and $2p_1$ cross sections at all energies.

Theoretical and experimental cross sections for elec-

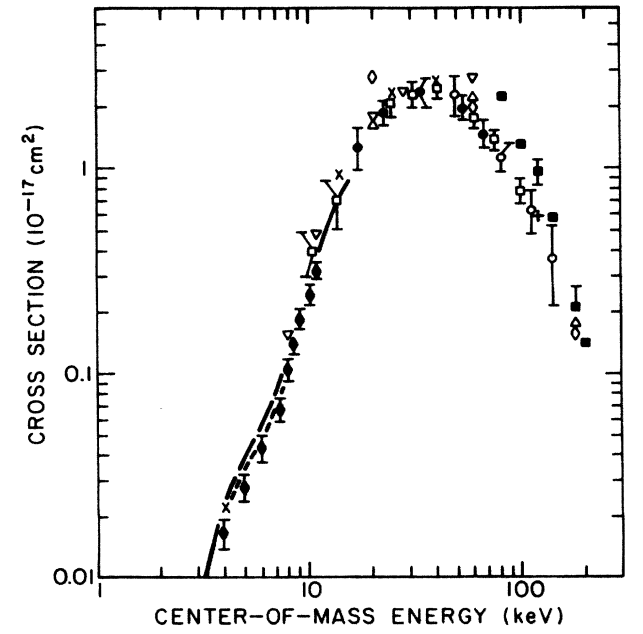

FIG. 12. Cross sections for electron transfer into all states of H in p-$^4He^+$ collisions. The theoretical results are labeled as in Fig. 9, with these changes: △, the double-center pseudostate results of Bransden *et al.* with basis *A* (Ref. 38); ■, the classical results of Olson (Ref. 52). The experimental results: ♦, Peart, Grey, and Dolder (Ref. 19); ●, Peart, Rinn, and Dolder (Ref. 20); □, Rinn *et al.* (Ref. 21); ○, Watts *et al.* (Ref. 22). The double-center pseudostate results of Fritsch and Lin (Ref. 25), which agree with the experimental and most theoretical results, have for clarity been omitted.

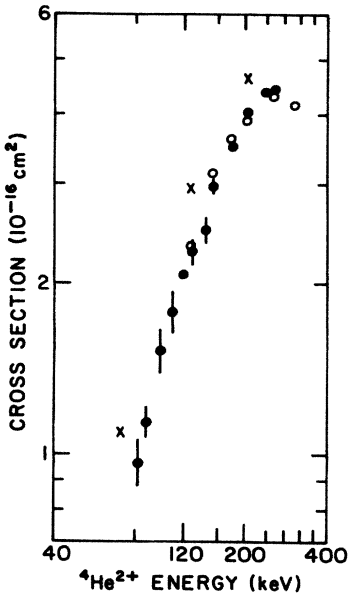

FIG. 13. Cross sections for ionization in He^{2+}-H collisions. ×, the present 34-state triple-center results. The experimental results: ○, Shah and Gilbody (Ref. 53); ●, Shah *et al.* (Ref. 54).

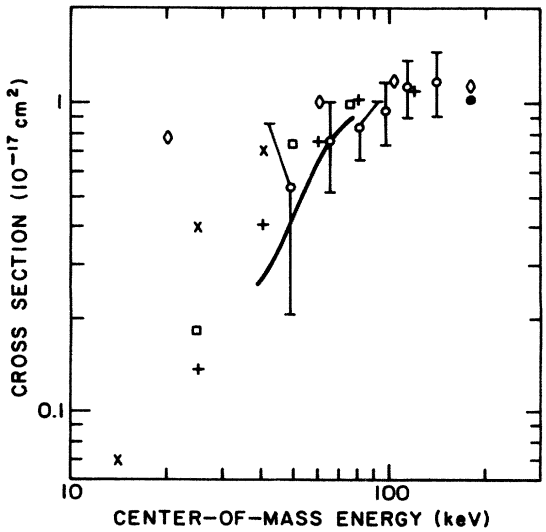

FIG. 14. Cross sections for ionization in p-He^+ collisions. Theoretical results: ×, the present 34-state triple-center results; +, the double-center Sturmian pseudostate results (Refs. 36 and 37); □, the double-center pseudostate results of Fritsch and Lin (Ref. 39); ◇, the one-and-a-half-center pseudostate results of Reading *et al.* (Ref. 41). The experimental data: ○, Watts *et al.* (Ref. 22); ●, Angel *et al.* (Ref. 23); ——, the experimental results of Peart, Rinn, and Dolder (Ref. 20).

tron transfer into all states of H in p-$He^+(1s)$ collisions are shown in Fig. 12. The experimental error limits in all cases are total error limits. Within these limits the experimental results are in accord. The triple-center results agree with the experimental results at all but the lowest common energy $E_{c.m.}=4$ keV, where the triple-center value is 12% above the upper error limit of Peart, Grey, and Dolder.[19] The plane-wave-factor molecular-state result,[5] the double-center pseudostate (AO +) result[25] (not shown), and the double-center Sturmian pseudostate result[24] are also somewhat above the error limit at this energy.

There are no coupled-state results for ionization in He^{2+}-H collisions other than the present triple-center results. Shown in Fig. 13 are these results and the two available sets of experimental results: those of Shah and Gilbody[53] and the recent lower-energy results of Shah, Elliott, and Gilbody.[54] (Only the random error limits are indicated in the latter measurements.) The triple-center results lie somewhat above the experimental results at all energies. Differences decrease from about 35% at the lowest energy to 10% at the highest energy. These differences, for ionization, are not large and may mainly reflect basis sensitivity noted in Sec. III A, which grows with *decreasing* energy.

Coupled-state and experimental cross sections for ionization in p-He^+ collisions are shown in Fig. 14. The error limits on the cross sections of Watts, Dunn, and Gilbody[22] are the estimated total error limits; error limits on the other data[20,23] are omitted. Even considering just the displayed error limits, the experiments are seen to be in accord. The triple-center result at the highest energy $E_{c.m.}=40$ keV lies above the experimental data, but is perhaps acceptably close, considering the large displayed error limits and the sensitivity to triple-center basis size. Experimental results at lower energies would be desirable.

ACKNOWLEDGMENTS

This work was supported by the U.S. Department of Energy, Office of Energy Research, Office of Basic Energy Sciences, Division of Chemical Sciences. All computations were performed on Pennsylvania State University's IBM 3090 computer.

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[43]As in previous work by the author and co-workers, Hamming's method (started by a Runge-Kutta integration) has been used; see Ref. 2 and references therein.

[44]For some very small probabilities of ionization in p-$He^+(1s)$ collisions at the energy $E_{c.m.}=4$ keV the change is up to 4%.

[45]For some small probabilities of capture or ionization, changes are up to 1%.

[46]At the lower energy $E_{c.m.}=4$ keV in p-$He^+(1s)$ collisions, the summed probability has been kept to unity within 1×10^{-6} to help maintain sufficient accuracy in the small ionization probability ($\lesssim 3\times10^{-4}$).

[47]At the lowest energy $E_{c.m.}=1.6$ keV, the summed probability is unity to within 1×10^{-5}, while the probability of electron transfer to $1s$ is very small ($\lesssim 6\times10^{-5}$); however, the other tests show that this transfer probability has a substantially greater absolute numerical accuracy than 1×10^{-5}.

[48]Cross sections of lesser accuracy are reported to only two significant figures.

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[50]To calculate the transition probabilities at one impact parameter with the 34-state basis, the required cpu time ranges from roughly 20 min at $E_{c.m.}=40$ keV to at least 30 min at $E_{c.m.}=4$ keV using an IBM 3090 computer at Pennsylvania State University.

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