PHYSICAL REVIEW A VOLUME 25, NUMBER 2 FEBRUARY 1982

Electron transfer in p-He$^+$ and He^{2+}-H collisions using a Sturmian basis

Thomas G. Winter
Physics Department, Pennsylvania State University, Wilkes-Barre Campus, Wilkes-Barre, Pennsylvania 18708

(Received 7 July 1981)

Total cross sections are reported for electron transfer into all bound states in colllisions of protons with ^{4}He$^+$ ions and ^{4}He^{2+} ions with H atoms at center-of-mass energies from 4 to 120 keV and 4 to 40 keV, respectively. The coupled-state calculations employ 19–24 Sturmian basis functions. Convergence of cross sections with respect to the size of this basis has been studied, and total cross sections are estimated to be converged to a few percent. A comparison is made with molecular-state, atomic-state, classical, and experimental results. In the energy region of overlap, Sturmian-state results and plane-wave-factor, molecular-state results agree to within 9% except for the p-He$^+$ process at 14 keV, where the Sturmian results are 37% larger, probably reflecting the need to include the continuum which was omitted in the molecular calculations. There is also a similar discrepancy with the experimental results of Peart, Grey, and Dolder; these Sturmian results, however, do tie in with the experimental results of Angel, Sewell, Dunn, and Gilbody at higher energies.

I. INTRODUCTION

Electron transfer in collisions between He^{2+} ions and H atoms and the "inverse process"—electron transfer in collisions between protons and He$^+$ ions—have been studied extensively in recent years both theoretically and experimentally. Being accidentally resonant and highly nonresonant, respectively, these one-electron processes may serve as two prototypes of electron transfer is not too asymmetric systems.

Studies on these processes have focused on the intermediate-energy range in which the projectile's speed is not very different from the speed of the orbital electron. In the lower part of this energy range, various coupled-molecular-state calculations have been carried out: perturbed-stationary-state calculations by Piacentini and Salin[1] (for the He^{2+}-H process only) and Winter, Hatton, and Lane[2–5]; plane-wave-factor, molecular-state calculations by Winter, Hatton, and Lane[3–5]; molecular-state calculations by Vaaben and Taulbjerg[6] (for the He^{2+}-H process only) using their own translational factors which are of Schneiderman-Russek type[7]; and molecular-state calculations by Kimura and Thorson[8] and Crothers and Todd[9] (for the He^{2+}-H process only) using optimized translational factors. In both parts of the energy range, coupled-atomic-state calculations have been carried out by Malaviya,[10] Msezane and Gallaher,[11] and Rapp,[12] and another atomic-state calculation (using a unitarized-distorted-wave method) has been carried out by Ryufuku and Watanabe[13] (for the He^{2+}-H process only). A very large coupled-state calculation with, however, only one state placed on the projectile nucleus (a "one-and-half-center" expansion) has recently been carried out by Reading, Ford and Becker.[14] In the upper portion of this energy range, classical calculations have been carried out by Olson, Salop, Phaneuf, and Meyer.[15–16]

It is hard to deal with the full intermediate-energy range using only one of these methods: In the bound-molecular-state approaches, more and more bound basis states become important as the energy is increased, the proper choice of translational factors becomes more important at the increasingly more important, larger impact parameters, and (in a not unrelated consideration) the molecular continuum may become important; these calculations have been restricted to center-of-mass energies of at most 14 keV. (For the ^{4}HeH^{2+} system, a center-of-mass energy of 20 keV corresponds to a projectile speed of 1 a.u. relative to the target, and to a ^{4}He^{2+} energy of 100 keV relative to the proton.) In the atomic-state approaches, as projectile speeds are decreased below 1 a.u., the atomic continuum may become more and more important for describing the molecular character of the electronic wave function during the collision, while at speeds much above 1 a.u. it becomes more and more important due to the increasing dominance of, and strong coupling to, ionization channels during the collision; despite these considerations, bound-atomic-state calculations have been carried out outside the "peak regions" where they might be hoped to be valid,[10–12] and must be subject to the test of experiment and more reliable calculations. The classical calculations have generally been limited to the higher-energy side of the intermediate-energy region.[15,16]

The problem of covering the energy range both somewhat below and above the "peak regions" was first addressed in the context of the proton-hydrogen electron-transfer process. Gallaher and Wilets[17] introduced a basis of Sturmian functions and Cheshire, Gallaher, and Taylor,[18] a basis of bound atomic states augmented by pseudostates. These bases each have the advantages of being square integrable and, in principle, complete. However, owing to their limited sizes, they were not really complete; the atomic continuum was only partially accounted for. (Eight Sturmian functions and 14 pseudostate-plus-atomic-state functions were included in the respective bases; limited tests of convergence of the Sturmian results were made by enlarging the basis.) Shakeshaft systematized and considerably enlarged the Sturmian calculations,[19,20] including up to 24*s* and *p* functions (12 centered on each nucleus) and, in one study, demonstrated *s*-state, but not *p*-state, convergence of cross sections. More recently, he modified the Sturmian functions slightly to form "scaled-hydrogenic" functions,[21] and carried out a very large calculation with 70 functions (35 centered on each nucleus). (Of course, owing to the nuclear symmetry for the p-H process, the N coupled equations fortunately decouple into two sets of $N/2$ coupled equations.)

The present Sturmian calculation is intended to treat the intermediate-energy range for the p-He^+ and He^{2+}-H electron-transfer processes. The Sturmian functions, as introduced by Gallaher and Wilets[17] and further described by Shakeshaft,[19] have the advantages of being systematic and simple, as well as square integrable: For each angular momentum l, they are simply exponentials with a single exponent $\exp[-Zr/(l+1)]$ multiplied by polynomials in r. (The nuclear charge is Z and the electron-nuclear separation is r.) (In addition to the previously cited work, systematic, fixed exponent bases have been successfully applied by Murtaugh and Reinhardt[22] to electron-atom scattering and, to a limited extent, by Winter and Lane[23] to electron-molecule scattering.) The basis is identical to that described by Shakeshaft, but since the evaluation of matrix elements differs from his method (Shakeshaft having used a variation of Cheshire's method[24] of simultaneously integrating differential equations for the charge-exchange matrix elements and the coefficients in the expansion of the electronic wave function), it seems worthwhile to describe the calculation in some detail.

The outline of the paper is as follows: In Sec. II, a review is given of the Sturmian basis functions and the coupled equations for the coefficients in the expansion of the electronic wave function, and the method of calculation of matrix elements and numerical checks are presented. In Sec. III, convergence studies for both electron-transfer processes are described, and their cross sections are presented and compared with other theoretical and with experimental results. Unless otherwise indicated, Hartree's atomic units are used throughout.

II. THEORY

A. Sturmian basis

Following Shakeshaft,[19] the time-dependent electronic wave function $\Psi(\vec{r},t)$ is expanded in approximate traveling atomic orbitals $f_{k\alpha}(\vec{r},t)$:

$$\Psi(\vec{r},t)=\sum_{k\alpha} a_{k\alpha}(t) f_{k\alpha}(\vec{r},t)\ , \tag{1}$$

where

$$f_{k\alpha}(\vec{r},t)=\psi_{k\alpha}[\vec{r}_\alpha(\vec{r},t)] \times\exp\left[-iE_{k\alpha}t\mp\frac{i\vec{v}\cdot\vec{r}}{2}-\frac{iv^2t}{8}\right]\ , \tag{2}$$

each $\psi_{k\alpha}$ being an approximate-atomic wave function (to be described below) centered on nucleus α (where α denotes nucleus $A=\mathrm{H}^+$ or $B=\mathrm{He}^{2+}$) with corresponding approximate eigenvalue $E_{k\alpha}$. The vectors $\vec{r}_\alpha$ and $\vec{r}$ are the position vectors of the electron in an inertial frame relative to the nucleus α and the midpoint of the internuclear line, respectively. The formulation, based on the formalism of Bates[25] in the context of an atomic basis, ensures that the matrix elements and coupled equations, and hence the cross sections obtained from them, are independent of the choice of origin on the internuclear line if the velocity $\vec{v}$ of nucleus B relative to nucleus A is constant. The upper or lower sign in the plane-wave factor $\exp(\mp i\vec{v}\cdot\vec{r}/2)$ is chosen according to whether $\alpha=A$ or B. The axis of quantization is chosen to be along $\vec{v}$.

The approximate-atomic-wave functions $\psi_{k\alpha}$ and eigenvalues $E_{k\alpha}$ are obtained by diagonalizing the atomic Hamiltonian

$$H_\alpha=\tfrac{1}{2}\nabla^2-\frac{Z_\alpha}{r_\alpha} \tag{3}$$

(Z_α being the charge of nucleus α) in a finite Sturmian basis $\varphi_{j\alpha}(\vec{r}_\alpha)$, $j=1,\ldots,j_{\max\alpha}$:

$$\langle\psi_{k\alpha}\,|\,H_\alpha\,|\,\psi_{k'\alpha}\rangle=E_{k\alpha}\delta_{kk'}\ , \tag{4a}$$

$$\langle\psi_{k\alpha}\,|\,\psi_{k'\alpha}\rangle=\delta_{kk'}\ , \tag{4b}$$

leading to the particular linear combinations

$$\psi_{k\alpha}=\sum_{j=1}^{j_{\max\alpha}}C_{kj\alpha}\varphi_{j\alpha}\ . \tag{5}$$

In the approach of Shakeshaft[19] just described, which is used in the present calculation, the electronic wave function Ψ in Eq. (1) has been expanded in terms of the approximate-atomic wave functions $\psi_{k\alpha}$, and the transition amplitudes are taken to be simply the coefficients $a_{k\alpha}$ at large positive times—i.e., the projections of Ψ onto *approximate*-atomic wave functions. Gallaher and Wilets,[17] on the other hand, expanded the electronic wave function Ψ directly in terms of the Sturmian functions $\varphi_{k\alpha}$, and obtained the transition amplitudes as projections of Ψ onto *exact*-atomic wave functions. There are unfortunately small but persistent oscillations in these amplitudes at large positive times. Shakeshaft[20] has noted, however, that both approaches yield variational estimates on the transition probability and that it is not obvious which one yields the more rapidly converging estimate as the size of basis is increased. It is perhaps more straightforward to use the approximate-atomic-state expansion at the outset, so that the expansion coefficients $a_{k\alpha}$ have direct physical significance. For example, one basis used in the present calculation consists of the 19 Sturmian functions $\varphi_{j\alpha}$ with corresponding approximate-atomic wave functions $\psi_{k\alpha}$ whose scaled eigenvalues $E_{k\alpha}/Z_\alpha^2$ are given in Table I. (The three labels are n, l, and m, referring to the principal, orbital, and magnetic quantum numbers, respectively.) (The choice of this particular basis is described in the convergence study in Sec. III A.) States having $n=l+1$ are exact, with $E_{nlm\alpha}=-Z_\alpha^2/(2n^2)$. For the particular basis chosen, the first two s states on either center are bound, the others representing portions of the continuum; as a further example, it might be noted that an additional Sturmian s state on nucleus B would add another bound state.

The Sturmian functions are defined by

$$\varphi_j(\vec{r})=S_{nl}(Z,r)\mathscr{Y}_{lm}(\hat{r})\ , \tag{6}$$

where

$$\mathscr{Y}_{lm}(\hat{r})=\begin{cases}Y_{lm}, & m=0\ ,\\ \dfrac{1}{\sqrt{2}}[Y_{lm}+(-1)^mY_{l-m}], & m>0\end{cases} \tag{7}$$

$$S_{nl}(Z,r)=Z^{3/2}\left[\frac{4(n-l-1)!}{n\,(l+1)^3(n+l)!}\right]^{1/2}\rho^l \times e^{-\rho/2}L_{n-l-1}^{2l+1}(\rho)\ , \tag{8a}$$

$$\rho=Z\frac{2r}{l+1}\ , \tag{8b}$$

TABLE I. Scaled eigenvalues using a 19-state Sturmian basis.

	E_{kA}/Z_A^2			E_{kB}/Z_B^2	
State kA	Approximate	Exact	State kB	Approximate	Exact
$1sA$	-0.5	-0.5	$1sB$	-0.5	-0.5
$2sA$	-0.07735	-0.125	$2sB$	-0.12217	-0.125
$3sA$	1.07735		$3sB$	0.04970	
			$4sB$	0.60926	
			$5sB$	4.12987	
$2p_{0,1}A$	-0.125	-0.125	$2p_{0,1}B$	-0.125	-0.125
			$3p_{0,1}B$	-0.05138	-0.05556
			$4p_{0,1}B$	0.10138	
			$3d_{0,1,2}B$	-0.05556	-0.05556

for arbitrary Z. For $Z=1$, the Sturmian function is as defined by Shakeshaft. The Laguerre polynomial $L_p^q(\rho)$ and the (real) modified spherical harmonic $\mathscr{Y}_{lm}$ are unchanged (except possibly for a different phase factor $(-1)^m$ which depends on the definition of the phase of the spherical harmonics Y_{lm}). Recurrence relations, differential equations, and orthonormality relations given by Shakeshaft must, of course, be changed to allow for arbitrary Z; these changes will be made as needed.

B. Coupled equations

Substituting the expansion for $\Psi(\vec{r},t)$ given by Eq. (1) into the time-dependent Schrödinger equation

$$\left[H-i\frac{\partial}{\partial t}\right]\Psi(\vec{r},t)=0\ ,$$

multiplying by a particular approximate traveling atomic orbital $f_{k\alpha}^*$ (the asterisk denoting complex conjugation), integrating over all space, and using the eigenvector-eigenvalue equations (4) determine coupled equations for the $a_{k\alpha}$'s. In vector form,

$$\underline{S}'(t)\frac{d\vec{a}(t)}{dt}=-i\underline{G}'(t)\vec{a}(t)\ , \tag{9}$$

where

$$[\vec{a}(t)]_{k\alpha}=a_{k\alpha}(t)\ , \tag{10}$$

$$\begin{aligned} S'_{k\alpha k'\beta}(t)&=\langle f_{k\alpha}(\vec{r},t)\,|\,f_{k'\beta}(\vec{r},t)\rangle \\ &=S_{k\alpha k'\beta}(t)P_{k\alpha k'\beta}(t)\ , \end{aligned} \tag{11}$$

$$\begin{aligned} G'_{k\alpha k'\beta}(t)&=\left\langle f_{k\alpha}(\vec{r},t)\left| H-i\frac{\partial}{\partial t}\right| f_{k'\beta}(\vec{r},t)\right\rangle \\ &=G_{k\alpha k'\beta}(t)P_{k\alpha k'\beta}(t)\ , \end{aligned} \tag{12}$$

$$P_{k\alpha k'\beta}(t)=\exp[i(E_{k\alpha}-E_{k'\beta})t]\ . \tag{13}$$

The overlap and coupling matrix elements $S_{k\alpha k'\beta}$ and $G_{k\alpha k'\beta}$ take two different forms. If $\alpha=\beta$, then they are called "direct" matrix elements:

$$S_{k\alpha k'\alpha}(t)=\delta_{kk'}\ , \tag{14}$$

$$G_{k\alpha k'\alpha}(t)=\left\langle \psi_{k\alpha}(\vec{r}_\alpha)\left| -\frac{Z_\beta}{r_\beta}\right| \psi_{k'\alpha}(\vec{r}_\alpha)\right\rangle . \tag{15}$$

If $\alpha\neq\beta$, then they are called "charge-exchange" matrix elements:

$$S_{k\alpha k'\beta}(t)=\langle \psi_{k\alpha}(\vec{r}_\alpha)\,|\,\exp(\pm i\vec{v}\cdot\vec{r})\,|\,\psi_{k'\beta}(\vec{r}_\beta)\rangle\ , \tag{16}$$

$$G_{k\alpha k'\beta}(t)=\left\langle \psi_{k\alpha}(\vec{r}_\alpha)\left|\exp(\pm i\vec{v}\cdot\vec{r})\left[H_\beta-E_{k'\beta}-\frac{Z_\alpha}{r_\alpha}\right]\right|\psi_{k'\beta}(\vec{r}_\beta)\right\rangle . \tag{17}$$

The upper or lower signs in Eqs. (16) and (17) are appropriate when $\alpha=A$ or B, respectively. The evaluation of the direct and charge-exchange matrix elements will be described in Sec. II C.

If the electron is assumed to be initially in a state labeled by $k\alpha=1s\alpha$ [where $\alpha=A$ ($=\mathrm{H}^+$) for the He^{2+}-H and B ($=\mathrm{He}^{2+}$) for the p-He^+ process], then the initial condition for which the coupled Eqs. (9) are to be solved is

$$a_{k'\beta}(-\infty)=\delta_{1s\alpha k'\beta}\ . \tag{18}$$

The probability for electron transfer into all bound states is

$$P(\rho)=\sum_{k=1}^{k^b_{\max\beta}}|a_{k\beta}(\infty)|^2 \tag{19}$$

for a given impact parameter ρ, where $\beta=B$ for the He^{2+}-H and A for the p-He^+ process and $k^b_{\max\beta}$ denotes the number of approximate bound-state wave functions on nucleus β.

As in previous work, the coupled equations have been integrated numerically with respect to the alternate variable vt using Hamming's method (started by a Runge-Kutta integration),[26] with the total absolute truncation error automatically being here kept between 10^{-4} and 10^{-6}. The accuracy of the integration of the coupled equations and the accuracy of the non-Hermitian parts of the charge-exchange matrix elements were sufficient to keep the total probability at unity to within 4×10^{-4} (and better than this except at the highest energies); probabilities for capture into all bound states should be numerically correct to at least three digits.

The total cross section for electron transfer into all bound states is obtained by integrating ρ times $P(\rho)$ [given by Eq. (19)]:

$$Q=2\pi\int_0^\infty d\rho\rho P(\rho)\ . \tag{20}$$

Simpson's rule has been used to an estimated accuracy of 1/2%.

Values of $\rho P(\rho)$ and Q for both the p-He^+ and He^{2+}-H processes are presented in Sec. III.

C. Matrix elements

Eqs. (15)–(17) for the direct and charge-exchange matrix elements are valid regardless of whether the atomic functions $\psi_{k\alpha}(\vec{r}_\alpha)$ are exact or approximate and, in the latter case, independently of the basis used to obtain them. Thus, they can serve as a starting point for either a conventional (exact) bound-atomic-state or a Sturmian-state approach. Both approaches are in fact taken here, and two similar sets of computer subroutines—each valid for any nuclear charge Z_α and any angular momentum $l \le 3$—have been written, one set for each approach. There are three reasons for writing the bound-atomic-state subroutines: (1) to check partially the similar Sturmian-state subroutines using readily available atomic-state results; (2) to check sometimes contradictory[11,12] atomic-state results for the presently considered processes; and (3) to provide a basis of comparison with Sturmian-state results for those processes for which bound-atomic-state results are not available. In what follows, however, only the Sturmian procedure will be described; the procedure for exact bound atomic states is similar, but simpler.

Substituting the Sturmian expansion, Eq. (5), into the Eqs. (15)–(17) for the matrix elements, one obtains the expressions

$$G_{k\alpha k'\alpha} = -Z_\beta \sum_{jj'} C_{kj\alpha} C_{k'j'\alpha} g_{jj'\alpha}, \quad \alpha = A,B \tag{21}$$

$$S_{kAk'B} = \sum_{jj'} C_{kjA} C_{k'j'B} s_{jAj'B} \;, \tag{22}$$

$$S_{k'BkA} = S^{*}_{kAk'B} \;, \tag{23}$$

$$\begin{aligned} G_{kAk'B} = {} & \sum_{jj'} C_{kjA} C_{k'j'B} \\ & \times [-Z_A g^{A}_{jAj'B} - Z_B (1 - z_{n'l'}) g^{B}_{jAj'B} \\ & + (\epsilon_{l'B} - E_{k'B}) s_{jAj'B}] \;, \end{aligned} \tag{24}$$

$$\begin{aligned} G_{k'BkA} = {} & \sum_{jj'} C_{kjA} C_{k'j'B} \\ & \times [-Z_B g^{B}_{jAj'B} - Z_A (1 - z_{nl}) g^{A}_{jAj'B} \\ & + (\epsilon_{lA} - E_{kA}) s_{jAj'B}]^{*} \;, \end{aligned} \tag{25}$$

where the direct Sturmian matrix elements are

$$g_{jj'\alpha} = \left\langle \varphi_{j\alpha}(\vec{r}_\alpha) \left| \frac{1}{r_\beta} \right| \varphi_{j'\alpha}(\vec{r}_\alpha) \right\rangle, \qquad \alpha = A,B, \;\; \beta = B,A \tag{26}$$

and the charge-exchange Sturmian matrix elements are

$$s_{jAj'B} = \langle \varphi_{jA}(\vec{r}_A) \,|\, \exp(i\vec{v}\cdot\vec{r}) \,|\, \varphi_{j'B}(\vec{r}_B) \rangle \;, \tag{27}$$

$$g^{\alpha}_{jAj'B} = \left\langle \varphi_{jA}(\vec{r}_A) \left| \exp(i\vec{v}\cdot\vec{r}) \frac{1}{r_\alpha} \right| \varphi_{j'B}(\vec{r}_B) \right\rangle, \qquad \alpha = A,B \;. \tag{28}$$

In Eqs. (24) and (25) the constants $z_{nl}, \epsilon_{l\alpha}$ are defined by

$$z_{nl} = \frac{n}{l+1} \;, \tag{29}$$

$$\epsilon_{l\alpha} = -\frac{Z_\alpha^2}{2(l+1)^2} \;. \tag{30}$$

In deriving Eqs. (24) and (25), one needs

$$H_\alpha \varphi_{j\alpha} = \left[-\frac{Z_\alpha (1 - z_{nl})}{r_\alpha} + \epsilon_{l\alpha} \right] \varphi_{j\alpha} \tag{31}$$

[where the atomic Hamiltonian H_α is defined by Eq. (3)], which follows from Shakeshaft's equations when generalized in Z_α.

1. *Direct Sturmian matrix elements*

The direct Sturmian matrix elements $g_{jj'\alpha}$ in Eq. (26) will now be evaluated. Defining $\vec{R}$ as the position vector of nucleus B with respect to nucleus A and using the addition theorem for spherical harmonics,[27] the generating function for Legendre polynomials,[27] and properties of the Clebsch-Gordan coefficients[27,28] $\langle l_1 l_2 m_1 m_2 \,|\, l_1 l_2 l m \rangle$, one finds

$$g_{jj'\alpha} = [(2l+1)(2l'+1)]^{1/2} \sum_{L=0}^{\infty} \frac{\langle l l' 0 0 \,|\, l l' L 0 \rangle}{(2L+1)^{3/2}} b_{l m l' m'}(\pm\hat{R})_0 f_{n l n' l' L}(Z_\alpha, R) \;, \tag{32}$$

where

$$b_{lml'm'}(\hat{R})=\begin{cases}\langle ll'mm' \mid ll'LM\rangle\sqrt{4\pi}\mathscr{Y}_{LM}(\hat{R}), & m \text{ or } m'=0\\ \frac{1}{\sqrt{2}}\langle ll'mm' \mid ll'LM\rangle\sqrt{4\pi}\mathscr{Y}_{LM}(\hat{R}) & \\ \qquad +\frac{i^{\,|M|-m-m'}}{c_{|M|}}\langle ll'm-m' \mid ll'LM\rangle\sqrt{4\pi}\mathscr{Y}_{l|M|}(\hat{R}), & m,m'\neq 0\end{cases} \tag{33}$$

[c_M being defined by Eq. (37)],

$$_qf_{nln'l'L}(Z_\alpha,R)=\int_0^\infty dr\, r^{q+2}S_{nl}(Z_\alpha,r) \times S_{n'l'}(Z_\alpha,r)\frac{r_<^L}{r_>^{L+1}}\,, \tag{34}$$

$$r_<,r_> = \text{lesser, greater of } r,R\,.$$

The upper, lower signs in $\pm\hat{R}$ correspond to $\alpha=A,B$. Using Condon and Shortley's definition of spherical harmonics,[27] and setting the polar and azimuthal angles of $\hat{R}$ to be

$$\Theta(=\cos^{-1}vt/R),\quad \Phi=\pi\,, \tag{35}$$

one finds

$$\sqrt{4\pi}\mathscr{Y}_{lm}(\hat{R})=c_m\left[(2l+1)\frac{(l-m)!}{(l+m)!}\right]^{1/2} \times P_{lm}(\cos\Theta)\,, \tag{36}$$

where

$$c_m=1 \text{ if } m=0 \text{ and } \sqrt{2} \text{ if } m>0 \tag{37}$$

and P_{lm} is an associated Legendre function. The radial integrals $_qf_{nln'l'L}$ can be calculated by upward recurrence in n and n' starting from

$$_qf_{l+1,l,l'+1,l',L}=\frac{2^{l+l'+2}(l+1)^{-l-2}(l'+1)^{-l'-2}}{Z_\alpha^{q-1}\mu^\lambda[(2l+1)!(2l'+1)!]^{1/2}} \times F_L(\lambda,\mu Z_\alpha R) \tag{38}$$

for each l,l',L and $q=0,\ldots,n_{\max}+n'_{\max}-l-l'-2$, where

$$\lambda=q+l+l'+2\,,$$
$$\mu=(l+1)^{-1}+(l'+1)^{-1}\,, \tag{39}$$

$$F_L(\lambda,p)=\int_0^\infty x^\lambda e^{-x}\frac{x_<^L}{x_>^{L+1}}\,, \tag{40}$$

$$x_<,x_> = \text{lesser, greater of } x \text{ and } p\,.$$

The recurrence relations for $_qf_{nln'l'L}$ connecting the indices q and n (or q and n') are readily derived from Shakeshaft's recurrence formula[19] for the radial Sturmian functions (after generalizing this formula in Z_α):

$$n\gamma^+_{n-1,l}S_{nl}=\left[\frac{\rho}{2}-n+1\right]S_{n-1,l} -(n-2)\gamma^-_{n-1,l}S_{n-2,l}\,, \tag{41}$$

where[19]

$$\gamma^\pm_{nl}=-\left[\frac{(n\mp l)(n\pm l\pm 1)}{4n(n\pm 1)}\right]^{1/2}. \tag{42}$$

For all cases for which n, $n'\leq 4$ and l, $l'\leq 1$, explicit formulas for the required radial integrals $_0f_{nln'l'L}$ have also been determined. For example,

$$_0f_{4s,4p,1}(Z,R)=-\frac{8320Z}{729\sqrt{30}w^2}\left[1-\left[1+w+\frac{w^2}{2}+\frac{517}{3120}w^3+\frac{127}{3120}w^4-\frac{97}{3120}w^5 +\frac{161}{4680}w^6-\frac{w^7}{117}+\frac{w^8}{1170}\right]\exp(-w)\right],$$

where $w=\mu ZR$. As a test values of f for these cases were calculated for $Z=1$, 2 at $R=0.1$, 1, 2, 20 using the recurrence relations, and compared with those calculated using the explicit formulas. The maximum relative difference is 5×10^{-6} except at $R=20$ for some exponentially decreasing (and hence negligible) f's.

2. *Charge-exchange Sturmian matrix elements*

To evaluate the charge-exchange matrix elements $s_{jAj'B}$ and $g^{\alpha}_{jAj'B}$ given by Eqs. (27) and (28), it is convenient to express the modified spherical harmonics $\mathscr{Y}_{lm}(\hat r_\alpha)$ in terms of those in the rotating (molecular) frame $\mathscr{Y}_{lm}(\hat r'_\alpha)$. For this purpose, rotation matrices are introduced. The definition of $D^{(l)}_{mm'}(\mathscr{R})$ is Rose's as stated in Refs. 27 and 29. If the $+z_\alpha$ axes are along $\vec v$ and the y_α axes are perpendicular to the collision plane, then the Euler angles (π,Θ,π) specify the orientation of the rotated axes with respect to the space-fixed axes; see also Eqs. (35). It can then be shown that

$$\mathscr{Y}_{lm}(\hat r_\alpha)=\sum_{m'\geq 0}(-1)^{m+m'}\tilde d^{(l)}_{mm'}(\Theta)\mathscr{Y}_{lm'}(\hat r'_\alpha)\ , \tag{43}$$

where

$$\tilde d^{(l)}_{mm'}(\Theta)=\begin{cases}\tilde d^{(l)}_{mm'}(\Theta), & m=m'=0\\ \sqrt{2}d^{(l)}_{mm'}(\Theta)\ , & \text{one of } m \text{ or } m'=0\ ,\\ d^{(l)}_{mm'}(\Theta)+(-1)^{m'}d^{(l)}_{m-m'}(\Theta), & m,m'>0\end{cases} \tag{44}$$

and where the D matrices have been replaced by d matrices

$$D^{(l)}_{mm'}[\mathscr{R}(\pi,\Theta,\pi)]=(-1)^{m+m'}d^{(l)}_{mm'}(\Theta)\ . \tag{45}$$

A general formula for these d matrix elements with $m\geq m'$ in terms of hypergeometric functions, and relations among d-matrix elements of different indices, are given in Ref. 29. All cases for $l\leq2$ have been checked against specific formulas given by Berman and Jacob.[30]

Hence,

$$s_{jAj'B}=\sum_{m_1m'_1\geq0}\tilde d^{(l)}_{mm_1}(\Theta)\tilde d^{(l')}_{m'm'_1}(\Theta)\times t_{j_1Aj'_1B}(v,\rho,vt)\ , \tag{46}$$

$$g^{\alpha}_{jAj'B}=\sum_{m_1m'_1\geq0}\tilde d^{(l)}_{mm_1}(\Theta)\tilde d^{(l')}_{m'm'_1}(\Theta)\times h^{\alpha}_{j_1Aj'_1B}(v,\rho,vt)\ , \tag{47}$$

where

$$t_{j_1Aj'_1B}(v,\rho,vt)=\int d\vec r\,'S_{nl}(Z_A,r'_A)\times\mathscr{Y}_{lm_1}(\hat r'_A)S_{n'l'}(Z_B,r'_B)\times\mathscr{Y}_{l'm'_1}(\hat r'_B)\exp(i\vec v\cdot\vec r)\ , \tag{48}$$

and h^{α} is the same except for the addition of a factor of r_α^{-1} in the integrand. Introducing spheroidal coordinates λ, μ, ϕ, one obtains

$$r'_\alpha=(\lambda\pm\mu)\frac{R}{2}\ , \tag{49}$$

$$\cos\theta'_\alpha=\frac{\lambda\mu\pm1}{\lambda\pm\mu}\ , \tag{50}$$

$$\vec v\cdot\vec r=\frac{v\rho}{2}\sqrt{(\lambda^2-1)(1-\mu^2)}\cos\phi+\frac{v^2t}{2}\lambda\mu\ , \tag{51}$$

where θ'_α is the (electronic) polar angle and where the upper, lower signs correspond to $\alpha=A,B$. Using Condon and Shortley's definition of spherical harmonics in Eq. (7), one then finds

$$t_{j_1Aj'_1B}(v,\rho,vt)=\frac{R^3}{16}(-1)^{m_1+m'_1}\left[(2l+1)(2l'+1)\frac{(l-m_1)!(l'-m'_1)!}{(l+m_1)!(l'+m'_1)!}\right]^{1/2}\times\int_1^\infty d\lambda\int_{-1}^{1}d\mu(\lambda^2-\mu^2)S_{nl}\left[\frac{R}{2}(\lambda+\mu)\right]S_{n'l'}\left[\frac{R}{2}(\lambda-\mu)\right]\times P_{lm_1}\left[\frac{\lambda\mu+1}{\lambda+\mu}\right]P_{l'm'_1}\left[\frac{\lambda\mu-1}{\lambda-\mu}\right]\exp\left[\frac{iv^2t}{2}\lambda\mu\right]I_{m_1m'_1}(x)\ , \tag{52}$$

where

$$x=\frac{v\rho}{2}[(\lambda^2-1)(1-\mu^2)]^{1/2}\ , \tag{53}$$

$$\begin{aligned}I_{mm'}(x)&=\int_0^{2\pi}d\phi\frac{c_m\cos m\phi}{\sqrt{2\pi}}\frac{c_{m'}\cos m'\phi}{\sqrt{2\pi}}\exp(ix\cos\phi)\\&=\frac{c_mc_{m'}}{2}[i^{m+m'}J_{m+m'}(x)+i^{|m-m'|}J_{|m-m'|}(x)]\ ,\end{aligned} \tag{54}$$

c_m being given by Eq. (37) and J_m being a Bessel function of the first kind.[28,31] The expression for $h^{\alpha}_{j_1Aj'_1B}(v,\rho,vt)$ is the same as for $t_{j_1Aj'_1B}(v,\rho,vt)$ in Eq. (52) except that the factor $[(\lambda\pm\mu)R]^{-1}$ is to be added to the integrand.

The real and imaginary parts of the double integrals over λ and μ have been evaluated numerically by Gauss-Laguerre integration over a variable depending on λ and Gauss-Legendre integration over μ. All functions S, P, J having common arguments at a given mesh point (λ,μ) have been evaluated by recurrence relations where possible. As the center-of-mass energy was increased from 4 to 120 keV, the number of integration points in λ and μ was increased from 8 and 16 to 16 and 20, respectively, to ensure the (at least) three-digit accuracy reported in Sec. II B. Since the charge-exchange matrix elements are not Hermitian, the probability conservation noted in that section is a good check on their correctness. Numerous checks were also made in the zero-velocity limit.

D. Numerical checks against previous results

By changing only two numbers inputted to the computer program (Z_B and the nuclear mass M_B), it could be run instead for the p-H process studied by Shakeshaft. In Ref. 19, he lists amplitudes for elastic scattering, excitation to the 2s state, and transfer to the individual 1s and 2s states at an energy of 25 keV and $\rho=1$ a.u. using a basis of $4-20$ s Sturmian functions symmetrically placed on the nuclei. Values for 4, 6, 12, 16, and 20 s Sturmian functions have been recalculated; for each, there is agreement to one unit in the third (last) reported digit. This is an excellent test of the s-state part of the program. In Ref. 20, Shakeshaft lists total cross sections for excitation and electron transfer at various energies using 12s and 12p functions (again symmetrically placed on the nuclei). At 25 keV, the total cross section for electron transfer to the ground state has been recalculated; there is agreement again to one unit in the third (last) reported digit. This is an excellent test of both the s- and p-state parts of the program. (The other individual-state cross sections were not calculated owing to the expense of the additional impact parameters required.)

Further tests were comparisons with available bound-atomic-state results; the majority of the subroutines used in the Sturmian calculations are also used in the bound-atomic-state calculations. The most exacting standard was found to be the four-state (1sA, 2sB, 2p_0B, 2p_1B) results of Malaviya[10] for the He^{2+}-H process. At a center-of-mass energy of 40 keV, the total cross sections for each of the three processes were recalculated; there is in each case agreement to one unit in the third digit. The agreement of these results lends further support to the belief that p states and the Z_α dependence have been included correctly.

For the p-He^+ and He^{2+}-H processes, large discrepancies have unfortunately been found with the eight-bound-atomic state (1$s\alpha$, 2$s\alpha$, 2$p_{0,1}\alpha$, $\alpha=A,B$) results of Msezane and Gallaher[11] and of Rapp,[12] both by the present author[32] and Bransden and Noble.[33] The latter results substantially agree, and will be reported in Sec. III.

Finally, a comparison was made at 25 keV with the eight-bound-atomic state (1$s\alpha$, 2$s\alpha$, 2$p_{0,1}\alpha$, $\alpha=A,B$) results of Cheshire, Gallaher, and Taylor[18] for the p-H process; the recalculated individual cross sections for excitation to the 2s and 2p states and electron transfer to the 1s, 2s, and 2p states all agree to at least 1%. the agreement with what should be identical results by Rapp, Dinwiddie, Storm, and Sharp[34] is not as good.

III. RESULTS

Using the coupled-Sturmian-state approach, total cross sections have been calculated for electron transfer into all states of H in p-$^4He^+$ collisions and all state of He^+ in $^4He^{2+}$-H collisions. These calculations were performed at the center-of-mass energies 4, 14, and 40 keV and, for the former process, 25, 60, and 120 keV as well. These total cross sections are shown in Tables II and III, respectively. (Also shown are some other theoretical results. Theoretical results will be compared in Sec. III B, and theoretical and experimental results, in Sec. III C.)

A. Convergence

For 4-, 14-, and 40-keV center-of-mass energies, probability times impact parameter $P(\rho)\rho$ is plotted versus impact parameter ρ in Figs. 1–3 for electron transfer into the ground state of H in p-$^4He^+$ collisions and in Figs. 4–6 for electron transfer into all states of He^+ in $^4He^{2+}$-H collisions, along with plane-wave-factor, molecular-state results at the lower two energies (and, for later comparison, eight-bound-atomic-state results). As in the previous molecular-state calculations, computing time is reduced by limiting calcuations to selected impact parameters when studying convergence with respect to the size of the basis. Usually these are values at which the $\rho P(\rho)$ have maxima. Although for both processes it is capture into all states which is of interest, for the p-$^4He^+$ process at the two lower energies it was sufficient to consider convergence for the ground-state process; at higher energies, for which capture into excited states becomes increasingly more important, one must consider convergence for capture into all states. (Based on Sturmian-state calculations at peak-impact parameters, capture into excited states contributes about 1, 10, and 20% at 4, 14, and 40 keV, respectively.) At the two lower energies, where molecular-state results are available, Sturmian-state and molecular-state peaks are approximately in phase, so the locations of the latter peaks could indicate at what impact parameters the convergence tests should be made. (See Figs. 1, 2, 4, and 5.)

At most energies for each process, the convergence of two types of bases was studied; a basis of the same functions centered on each nucleus (except, of course, for different Z_α's), and a basis of different functions centered on each nucleus. (See Tables IV and V, respectively.) The most complete tests were carried out at 14 keV. Obviously, for symmetric systems such as $H_2{}^+$, symmetric bases are appropriate; for simplicity, "symmetric bases" might be carried over to the HeH^{2+} system.

Consider first the symmetric bases and, in particular, the contributions from s states. For the ground-state, p-$^4He^+$ process, the 6s state(s) have at most a 2% effect in a strictly s-state basis. (At 60 keV, the effect is 8% when capture into excited states—important at higher energies—is also included.) (Note that the changes generally oscillate as more and more states are added.) The effect, however, is less than 1% if the basis already has

TABLE II. Cross sections (in units of Å^2) for electron transfer in p-$^4He^+$ collisions using bases of Sturmian, bound molecular, and bound atomic states at various center-of-mass energies E.

Type of basis	Number of functions	Authors	Capture state(s)[a]	E(keV)=4	8	14	25	40	60	120
Molecular *pss*	10	Winter, Hatton, and Lane	1s =all	0.00183	0.0102	0.0576				
Molecular with plane wave factors	10	Winter, Hatton, and Lane	1s =all	0.00228	0.0124	0.0716				
Molecular with optimized translational factors	10	Kimura and Thorson	1s all	0.00194 0.00199	0.00889 0.00985					
Atomic	8	Msezane and Gallaher	1s	0.256	0.237			0.077		
Atomic	8	Rapp	1s			0.11[b]		0.169		0.039
Atomic	8	Bransden and Noble	1s	0.0018[b]		0.040		0.152		0.043[b]
Atomic	8	Winter (this work)	1s	0.00170		0.0400		0.155		0.0443
Atomic	8	Bransden and Noble	all	0.0023[b]		0.048[b]		0.16[b]		0.049[b]
Sturmian	19–24[c]	Winter (this work)	1s	0.00211		0.0917	0.213	0.235	0.172	0.0452
			all			0.0979	0.233	0.268	0.207	0.0611

[a] Cross sections marked "all" are for capture into all *available* bound states.

[b] Graphically interpolated values.

[c] The 19 states 1sA, 2sA, 3sA, $2p_{0,1}A$, 1sB,..., 5sB, $2p_{0,1}B$,..., $4p_{0,1}B$, $3d_{0,1,2}B$ at 14 keV; the 21 states consisting of these 19 states plus $5p_{0,1}B$ at 4 keV; and the 24 states 1$s\alpha$,..., 6$s\alpha$, $2p_{0,1}\alpha$, $\alpha=A$, B, $3p_{0,1}B$,..., $6p_{0,1}B$ for $E\geq 25$ keV.

TABLE III. Total cross sections (in units of Å^2) for electron transfer into all states of He$^+$ in ^{4}He^{2+}-H collisions at various ^{4}He^{2+} laboratory energies E using a basis of Sturmian, bound molecular, and bound atomic states.

Type of basis	Number of functions	Authors	E(keV) = 20	40	70	200
Molecular *pss*	3	Piacentini and Salin	5.34			
Molecular *pss*	20	Winter and Lane	9.37			
Molecular *pss*	22	Hatton, Lane and Winter	9.31			
Molecular with plane-wave factors	10	Hatton, Lane and Winter	12.2	13.5	12.1	
Molecular with optimized translational factors	10	Kimura and Thorson	11.23			
Molecular with optimized translational factors	5	Crothers and Todd	13[b]			
Molecular with Schneiderman-Russek type factors	14	Vaaben and Taulbjerg	9.63			
Atomic	8	Msezane and Gallaher	11.7	9.93		1.52
Atomic	8	Rapp	12[b]	12[b]		2.29
Atomic	8	Bransden and Noble	10[b]	12[b]	9.84	2.19
Atomic	8	Winter (this work)	10.1		9.92	2.21
Atomic	$8+(n\geq 3)$[a]	Bransden and Noble	10[b]	12[b]	11.52	4.01
Sturmian	$19-24$[c]	Winter (this work)	11.1		11.0	3.74

[a] Capture cross sections including estimated contributions from states with $n\geq 3$ by Bransden, Newby, and Noble (Ref. 36).

[b] Graphical or interpolated values.

[c] The 19 states $1sA$, $2sA$, $3sA$, $2p_{0,1}A$, $1sB,\ldots$, $5sB$, $2p_{0,1}B,\ldots$, $4p_{0,1}B$, $3d_{0,1,2}B$ at 70 keV; the 21 states consisting of these 19 states plus $5p_{0,1}B$ at 20 keV; and the 24 states $1s\alpha,\ldots$, $6s\alpha$, $2p_{0,1}\alpha$, $\alpha=A$, B, $3p_{0,1}B,\ldots$, $6p_{0,1}B$ at 200 keV.

some p states. These state(s) are neglected except at energies of at least 25 keV. For the He^{2+}-H process, even though p states serve greatly to damp the s-state oscillations, higher s states are somewhat more important, since capture into the $2s$ and higher states is important. At 14 keV, neglecting the $6s$ state is a 2% effect. (A test at 40 keV using a nonsymmetric basis indicates that the $7sB$ state has a 3% effect; see Table V.) The slower s-state convergence for the ^{4}He^{2+}-H process is one reason why their cross sections above 40 keV are not reported.

Consider now p-state convergence, still within

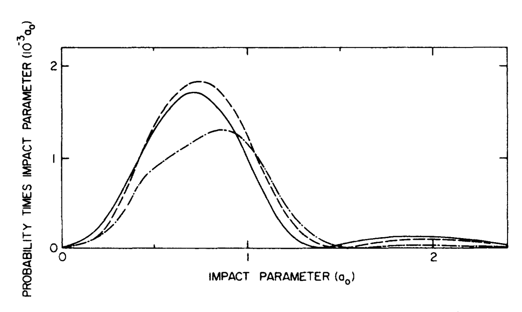

FIG. 1. Probability times impact parameter for electron transfer to the ground state of H in 4-keV, p-^{4}He$^+$ collisions. Solid curve, 21-Sturmian-state result (this work); dashed curve, ten-molecular-state result with plane-wave factors of Winter, Hatton, and Lane (Ref. 5); dash-dotted curve, eight-bound-atomic-state result (this work).

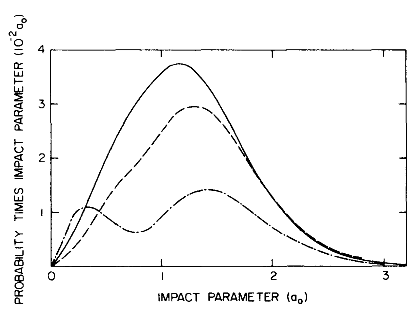

FIG. 2. Probability times impact parameter for 14-keV, p-^{4}He$^+$ collisions. The curves are as in Fig. 1, except that the solid curve is a 19-Sturmian-state result.

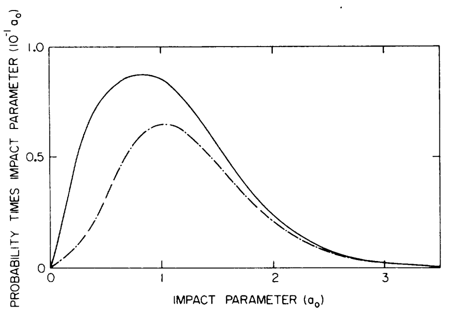

FIG. 3. Probability times impact parameter for 40-keV, p-^{4}He$^+$ collisions. The curves are as in Fig. 1, except that the solid curve is a 24-Sturmian-state result.

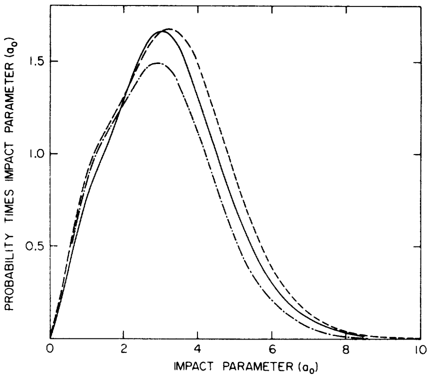

FIG. 5. Probability times impact parameter for 14-keV, ^{4}He^{2+}-H collisions. The curves are as in Fig. 4, except that the solid curve is a 19-Sturmian-state result.

the confines of a "symmetric" basis. for the p-^{4}He$^+$ process at 4 and 14 keV, the 5p states have a 2% and 1% effect, respectively, and at 40 and 60 keV, the 6p states have a 1% and 5% effect, respectively. States up to 5p and 4p were retained at 4 and 14 keV, respectively, and states up to 6p were retained at higher energies. (Additional tests at 14 keV, made after total cross sections were calculated, unfortunately showed that the 5p, 6p, and 7p states are all contributing in the positive direction; at this energy, these states may *raise* the cross section by about 4%.) For the ^{4}He^{2+}-H process, the 5p states have no larger an effect at 4 and 14 keV than for the p-^{4}He$^+$ process, but at 40 keV the 6p states have a larger (11%) effect than for the other process; nonetheless, the same basis was used for this process, in light of an additional test using a nonsymmetric basis. [The $7p_{0,1}B$ states were found to produce only a 4% effect (not shown in Table V), and of opposite sign.]

Since the number of s and p states retained so far is already large (up to 32), the number of states centered on nucleus A ($=$H$^+$) will be reduced before considering the effect of d states. It is reasonable to consider states centered on nucleus A to be less important since, for a given principal quantum number, they have a higher energy. Referring to Table V, it is seen that for the p-^{4}He$^+$ process at the lower two energies, the combined effect of the 5 states $4sA$, $3p_{0,1}A$, $4p_{0,1}A$ is only 1%, while at 40 and 60 keV the combined effect of the states $3p_{0,1}A$, $4p_{0,1}A$, $5p_{0,1}A$ is also 1%. At 60 keV, the $4sA$ state has a significant effect (7%) when capture into excited states is also included. For the ^{4}He^{2+}-H process, the combined effect of the states $4sA$, $3p_{0,1}A$, $4p_{0,1}A$, and (at 40 keV) $5p_{0,1}A$, $6p_{0,1}A$

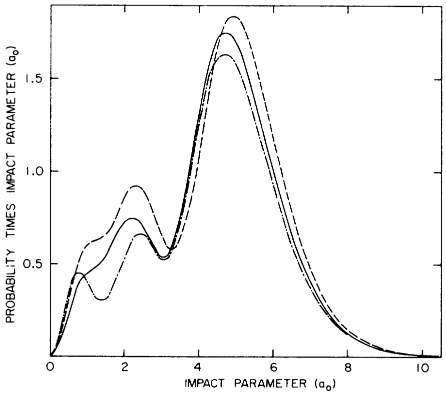

FIG. 4. Probability times impact parameter for electron transfer to all states of He$^+$ in 4-keV (c.m.), ^{4}He^{2+}-H collisions. Solid curve, 21-Sturmian-state result (this work); dashed curve, ten-molecular-state result with plane-wave factors of Winter and Hatton (Ref. 4); dash-dotted curve, eight-bound-atomic-state result (this work).

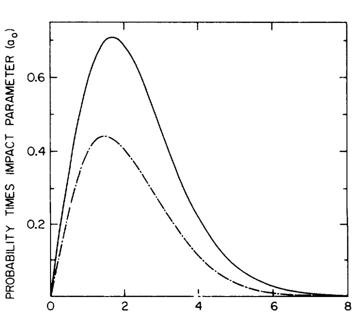

FIG. 6. Probability times impact parameter for 40-keV ^{4}He^{2+}-H collisions. The curves are as in Fig. 4, except that the solid curve is a 24-Sturmian-state result.

is larger (3 — 5 %) at peak-impact parameters, but these states have still been neglected to keep the basis from being untractibly large. The effect of the $3d_{0,1,2}B$ states on the p-^{4}He$^+$ and ^{4}He^{2+}-H probabilities is at most 1% and 3%, respectively; these states were retained except for the former process at energies of at least 14 keV, although they are in fact no more important than the previously neglected states $4sA$, $3p_{0,1}A, \ldots$. For both processes, tests at 14 keV show that the $4d_{0,1,2}B$, $5d_{0,1,2}B$ states and the $3d_{0,1,2}A$, $4d_{0,1,2}A$, $5d_{0,1,2}A$ states (some of which are in the continuum) contribute at most 1%, and have therefore been neglected. Also shown are additional values which indicate that higher lying sB states are probably not important.

B. Comparison of theoretical results

Compare first the Sturmian- and molecular-state results. The overlapping center-of-mass energies are 4 and 14 keV, equivalent to ^{4}He^{2+} energies of 20 and 70 keV, respectively, relative to a stationary proton. Referring to Table III and Fig. 8 for the ^{4}He^{2+}-H process, it is seen that in cross sections, the present Sturmian- and the plane-wave-factor, molecular-state results of Hatton, Lane, and Winter[3] and Winter and Hatton[4] differ by only 9% at either energy, the Sturmian results being lower. Further, referring to Figs. 4 and 5, it is seen that the results also agree fairly closely in their impact-parameter dependence. This agreement holds at the peak-impact parameters; the less good agreement at other impact parameters may reflect a deficiency in either basis there (recall that the convergence of the Sturmian bases was monitored and controlled mostly at the principal peaks, which mainly determine the areas under the curves). The agreement in total cross sections is well within the previously estimated[4] 15% convergence of the molecular-state values. Also shown in Table III and Fig. 8 is the recent ten-molecular-state cross section of Kimura and Thorson[8] using optimized translational factors; the agreement at the single overlapping ^{4}He^{2+} energy of 20 keV is outstanding (within 1%). (This energy is the high-energy limit of all the tabulated molecular-state results except those using plane-wave factors.) The 16% agreement with the recent five-molecular-state results of Crothers and Todd[9] using optimized translational factors is fair. However, the latter results do not agree very well with either the plane-wave-factor results of Hatton *et al.*[3] or the optimized-translational-factor results of Kimura and Thorson[8] at lower energies which enjoy close agreement (within at least 4%) among themselves. The reason for this disagreement at the lower energies is unclear. Regarding the results of Vaaben and Taulbjerg,[6] Kimura and Thorson[8] have remarked on their own inability to reproduce these results using the same approximation as Vaaben and Taulbjerg have supposedly used; further, at lower energies (not shown in Table III), the results of Vaaben and Taulbjerg agree poorly with all the other molecular-state results except those of Crothers and Todd (with which they disagree at higher energies).

The Sturmian- and molecular-state results for the p-^{4}He$^+$ process will now be compared. (Atomic-state results for both processes will be considered later in this section.) Referring to Table II, it is seen that at the lowest center-of-mass energy (4 keV), the Sturmian-state cross section agrees well with both the plane-wave-factor, molecular, molecular-state result[5] and the optimized-translational-factor, molecular-state result,[8] being below the former by 7% and above the latter by 6%; further, the agreement in impact-parameter dependence in the former case (displayed in Fig. 1) is also good. Unfortunately, the agreement with the plane-wave-factor, molecular-state result vanishes at 14 keV: The Sturmian-state result is 28% higher if capture into only the ground state is considered (and 37% higher if capture into all *available* bound states is considered). This is disturbing, and suggests that the moelcular-state result is not converged at the higher energy, perhaps due to the neglect of coupling with the continuum. The previously noted study of convergence for the Sturmian basis suggests that adding to this basis would tend to *raise* the Sturmian cross section only slightly. A further discussion of this discrepancy will be made below when the bound-atomic-state results are described.

Eight-bound-atomic-state cross sections due to Msezane and Gallaher[11] and Rapp[12] are available for both processes for a comparison with the present Sturmian-state results. However, these bound-atomic-state cross sections are probably in error.[35] They have been recalculated independently by Bransden and Noble[33] and by the present author.[32] The recalculated values given in Tables II and III agree closely: within 2% or one unit in the last digit; they disagree greatly with several values of Refs. 11 and 12, also given in the tables. (Bransden and Noble also tabulate values at

TABLE IV. Probability times impact parameter ρ for electron transfer[a] in p-^{4}He$^+$ and ^{4}He^{2+}-H collisions at various center-of-mass energies, calculated using a "symmetric" basis of Sturmian functions centered on each nucleus (the subscripts specifying the centers therefore here being omitted).

	p-^{4}He$^+$ process				^{4}He^{2+}-H process			
	E(keV)=4	14	40	60	4	14	14	40
Basis functions	$\rho(a_0)$=0.7	1.4	1	0.75	5	1.4	3.2	1
$1s,2s,3s$[b]		0.0343	0.1078	0.1099		0.599		0.325
$+4s$	0.00157	0.0361	0.0993	0.0856	0.084	0.359		0.240
$+5s$	0.00164	0.0366	0.1006	0.0820	0.153	0.305		0.203
$+6s$	0.00167	0.0362	0.1016	0.0894	0.157	0.464		0.346
$+7s$		0.0363		0.0877		0.443		
$1s,2s,3s,4s,$ $2p_{0,1},3p_{0,1}$		0.0304	0.0749			1.016		0.583
$+5s$		0.0310	0.0755			0.959	1.623	0.554
$+6s$		0.0310	0.0756			0.996	1.649	0.685
$1s,2s,3s,4s$	0.00157	0.0361	0.0993		0.084	0.359		0.240
$+2p_{0,1}$	0.00137	0.0262	0.0865		1.475	1.081		0.410
$+3p_{0,1}$	0.00145	0.0304	0.0749		1.563	1.016		0.583
$+4p_{0,1}$	0.00164	0.0339	0.0779		1.609	1.004		0.447
$+5p_{0,1}$	0.00167	0.0344	0.0856	0.0717	1.609	0.996		0.461
$+6p_{0,1}$		0.0350	0.0868	0.0758		1.009		0.516
$+7p_{0,1}$		0.0353				0.994		

[a] The electron transfer is into all states except for the p-^{4}He$^+$ process at 4, 14, and 40 keV, where the rate of convergence is approximately determined by the rate for the ground-state process.

[b] In a given row, the basis in each group consists of all functions listed down to and including those in that row. (The last basis consists of 32 functions: 16 functions $1s,\ldots,4s$, $2p_0$, $2p_1,\ldots,7p_0$, $7p_1$ centered on each nucleus.)

numerous other energies, and display individual-state cross sections.)

For the ^{4}He^{2+}-H process at the lower three energies in Table III, the recalculated, eight-bound-atomic-state cross section enjoys good agreement with the Sturmian-state cross section, being *below* the Sturmian value by about 10%. (See also the impact-parameter dependence in Figs. 4 and 5.) (Bransden and Noble have also noted surprisingly good agreement with molecular-state results at the lower energies.) By the highest displayed energy (200 keV), however, the eight-bound-atomic-state method has failed: The total cross section (in Table III) and $P(\rho)\rho$ (in Fig. 6) are too low. Bransden, Newby, and Noble[36] have noted that at higher energies such as this, there is significant capture into He$^+$ states with $n \geq 3$. They have included this contribution by means of two-state calculations, and their corrected value at 200 keV (noted in Table III) agrees closely with the Sturmian-state result (within 7%).

For the p-He$^+$ process, the recalculated eight-bound-atomic-state cross section agrees well (within 10%) with the corresponding Sturmian-state value at the lowest energy. However, it is a factor of 2 too low at 14 keV and 20% too low at 120 keV, which for this process would suggest the considerable importance of the (atomic) continuum at these energies. In two preliminary calculations, Bransden and Noble[33] and Fritsch and and Lin[37] have recently noted that other pseudostate bases also raise this cross section over its value obtained when only bound atomic states are included.

Shown in Figs. 7 and 8 (along with some other previously considered theoretical results, and experimental results to be compared with in the next section) are the recent results of Reading, Ford, and Becker[14] using a very large basis of 54 states on one nucleus but only one state on the other nucleus (a "one-and-a-half-center" expansion). (Omitted from Fig. 7 at 60.4 keV for clarity is their point which is nearly coincident with the Sturmian

TABLE V. Probability times impact parameter ρ for electron transfer[a] in p-^{4}He$^+$ and ^{4}He^{2+}-H collisions at various center-of-mass energies, calculated using a "nonsymmetric" basis of Sturmian functions.

	p-^{4}He process				^{4}He^{2+}-H process				
	E(keV)=4	14	40	60	4	14	14	40	40
Basis functions	$\rho(a_0)$=0.7	1.4	1	0.75	5	1.4	3.2	1	1.5
14 or 18 functions[b,c]		0.0336				1.052			
$+3sA$	0.00162	0.0343	0.0857	0.0802	1.555	0.974	1.582	0.525	
$+4sA$			0.0862	0.0753				0.501	
$+3p_{0,1}A+4p_{0,1}A$	0.00164	0.0339			1.609	1.004	1.657		
$+5p_{0,1}A+6p_{0,1}A$			0.0868	0.0758				0.516	
(14 or 18 functions)[c]$+3sA$	0.00162	0.0343	0.0857[d]	0.0753[d]	1.555	0.974	1.582	0.501[d]	
$+3d_{0,1,2}B$	0.00160	0.0339	0.0858[d]	0.0753[d]	1.596	1.033	1.637	0.509[d]	
$+5sB$		0.0340				0.987			
$+4d_{0,1,2}B$		0.0338				1.000			
$+5d_{0,1,2}B$		0.0339				0.995			
14 functions[c]$+3sA$		0.0343				0.974			
$+3d_{0,1,2}A,\ldots,5d_{0,1,2}A$		0.0340				0.966			
18 functions[c]$+3sA+4sA+3d_{0,1,2}B$			0.0858					0.509	0.643
$-4sA+5sB+6sB$			0.0852					0.593	0.701
$+7sB$									0.681

[a] The electron transfer is into all states except for the p-He$^+$ process at 4, 14, and 40 keV, where the rate of convergence is approximately determined by the rate for the ground-state process.

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

[c] The 14 functions $1sA$, $2sA$, $2p_{0,1}A$, $1sB$, ..., $4sB$, $2p_{0,1}B$, ..., $4p_{0,1}B$ at 4 and 14 keV and the 18 functions = preceding 14 functions + the 4 functions $5p_{0,1}B$, $6p_{0,1}B$ at 40 and 60 keV.

[d] The $4sA$ function is also included.

result.) Considering the magnitude of each calculation, the overall agreement in the energy dependence between the two sets of results does not appear to be good for either process. Reading *et al.* have suggested a possible lack of convergence of their basis. It is to be noted, further, that for the p-He$^+$ process a large part of the discrepancy may be due to their assumption of an n^{-3} rule for summing over the excited capture states, which may not be valid at these energies; the ground-state capture cross sections agree well except at their lowest energy.[14]

Also shown in Figs. 7 and 8 are the classical results of Olson[15] and Olson *et al.*[16] The agreement between these results and the Sturmian-state results is fairly good for the He^{2+}-H process at higher energies; for the p-He$^+$ process at ~ 120 keV, Olson's value (with error limits included) is above the Sturmian value.

Not shown are the unitarized-distorted wave results of Ryufuku and Watanabe[13] for the He^{2+}-H process, which agree roughly with the other theoretical data at the intermediate energies.

C. Comparison with experimental results

The experimental results of Peart, Grey, and Dolder[38] and of Angel, Dunn, Sewell, and Gilbody[39] and Angel, Sewell, Dunn, and Gilbody[40] for the p-He$^+$ process shown in Fig. 7 include both the estimated random and systematic errors. The lower-energy data of Refs. 38 and 39 are for capture plus ionization, but the ionization cross section is probably small at these energies.[40] At the lowest energy (4 keV) of the Sturmian results, the

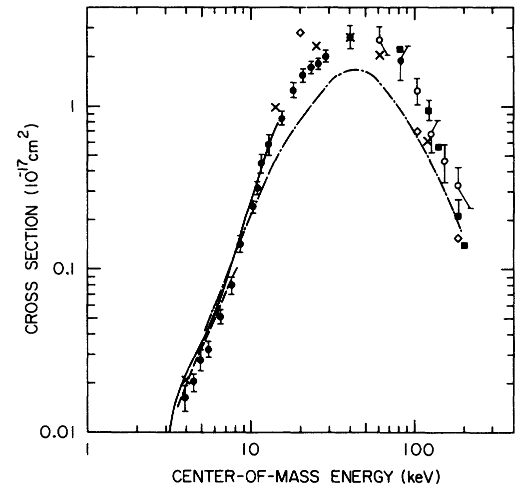

FIG. 7. Cross sections for electron transfer into all states of He$^+$ in p-^{4}He$^+$ collisions. The theoretical results: ×, the present 19- to 24-Sturmian-state results;—, the 10-molecular-state results with plane-wave factors of Winter *et al.*, Ref. 5; — — —, the 10-molecular-state results of Kimura and Thorson with optimized translational factors, Ref. 8; —·—·—·, the 8-atomic-state results of Bransden and Noble, Ref. 33; ◇, the "one-and-a-half-center," coupled-state results of Reading *et al.*, Ref. 14; ■, the classical results of Olson, Ref. 15. The experimental data: ●, Peart *et al.*, Ref. 38; ○, Angel *et al.*, Refs. 39 and 40.

Sturmian result lies 7% above the upper error bar of Peart *et al.* At the next two higher energies (14 and 25 keV), the Sturmian results lie significantly (20%) above the upper error bars of Peart *et al.* At the last three energies (40, 60, and 120 keV), however, the Sturmian results do lie between the error bars of Angel *et al.*[39,40] Since the Sturmian results appear to be converged well within 10% and since, if anything, they should be *raised* at 14 keV (recalling the convergence test in Sec. III A), the discrepancy with the data of Peart *et al.* at their higher energies is unresolved. It might be noted that the higher energy data of Peart *et al.*, if extrapolated towards the cross section's maximum, appear to be somewhat displaced from the other data.

The experimental results of Shah and Gilbody[41] (and Nutt, McCullough, Brady, Shah, and Gilbody[42] at the lower energies) and of Bayfield and Khayrallah[43] for the He^{2+}-H process shown in Fig. 8 also include both the estimated random and systematic errors. Also shown are the experimental data of Olson, Salop, Phaneuf, and Meyer[16] The Sturmian results are in excellent agreement with the data of Shah and Gilbody and Olson *et al.* at all energies; they are somewhat below the lower error bars of Bayfield and Khayrallah.

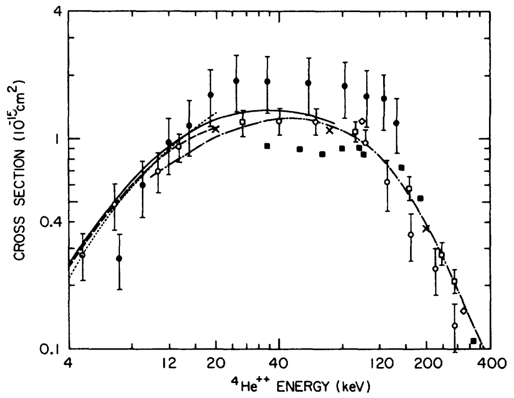

FIG. 8. Cross sections for electron transfer into all states of He$^+$ in ^{4}He^{2+}-H collisions. The theoretical results: ×, the present 19- to 24-Sturmian-state results; ——, the 10-molecular-state results with plane-wave factors of Hatton *et al.*, Ref. 3; — — —, the 10-molecular-state results of Kimura and Thorson with optimized translational factors, Ref. 8; · · · , the 5-molecular-state results of Crothers and Todd with optimized translational factors, Ref. 9; —·—·—·, the atomic-state results of Bransden and Noble, Ref. 33; ◇, the "one-and-a-half-center," coupled-state results of Reading *et al.*, Ref. 14; ■, the classical results of Olson *et al.*, Ref. 16. The experimental data: ○, Shah and Gilbody, Ref. 41 (^{3}He^{2+}), and Nutt *et al.*, Ref. 42 (^{3}He^{2+}); ●, Bayfield and Khayrallah, Ref. 43; □, Olson *et al.*, Ref. 16 (^{3}He^{2+}). The data noted are for ^{3}He^{2+} projectiles at velocities equivalent to those for ^{4}He^{2+} projectiles.

ACKNOWLEDGMENTS

All calculations were performed on Pennsylvania State University's IBM 3033 computer. The author would like to thank the Physics Department of Kansas State University for its hospitality during summer visits when this work was supported by the U. S. Department of Energy. He is also grateful to W. R. Thorson, D. S. F. Crothers, and A. L. Ford for preprints of their papers.

[1] R. D. Piacentini and A. Salin, J. Phys. B 7, 1666 (1974); 9, 563 (1976); 10, 1515 (1977).

[2] T. G. Winter and N. F. Lane, Phys. Rev. A 17, 66 (1978).

[3] G. J. Hatton, N. F. Lane, and T. G. Winter, J. Phys. B 12, L571 (1979).

[4] T. G. Winter and G. J. Hatton, Phys. Rev. A 21, 793 (1980).

[5] T. G. Winter, G. J. Hatton, and N. F. Lane, Phys. Rev. A 22, 930 (1980).

[6] J. Vaaben and K. Taulbjerg, *Abstracts of Papers, Eleventh International Conference on the Physics of Electronic and Atomic Collisions, Kyoto, Japan, 1979* (The Society for Atomic Collision Research, Kyoto, 1979), p. 566.

[7] S. B. Schneiderman and A. Russek, Phys. Rev. 181, 311 (1969); J. Vaaben and K. Taulbjerg, J. Phys. B 14, 1815 (1981).

[8] M. Kimura and W. R. Thorson, Phys. Rev. A 24, 3019 (1981).

[9] D. S. F. Crothers and N. R. Todd, J. Phys. B 14, 2251 (1981).

[10] V. Malaviya, J. Phys. B 2, 843 (1969).

[11] A. Msezane and D. F. Gallaher, J. Phys. B 6, 2334 (1973).

[12] D. Rapp, J. Chem. Phys. 61, 3777 (1974).

[13] H. Ryufuku and T. Watanabe, Phys. Rev. A 18, 2005 (1978).

[14] J. F. Reading, A. L. Ford, and R. L. Becker (unpublished); A. L. Ford (private communication).

[15] R. E. Olson, J. Phys. B 11, L227 (1978).

[16] R. E. Olson, A. Salop, R. A. Phaneuf, and F. W. Meyer, Phys. Rev. A 16, 1867 (1977).

[17] D. F. Gallaher and L. Wilets, Phys. Rev. 169, 139 (1968).

[18] I. M. Cheshire, D. F. Gallaher, and A. J. Taylor, J. Phys. B 3, 813 (1970).

[19] R. Shakeshaft, J. Phys. B 8, 1114 (1975).

[20] R. Shakeshaft, Phys. Rev. A 14, 1626 (1976).

[21] R. Shakeshaft, Phys. Rev. A 18, 1930 (1978).

[22] T. S. Murtaugh and W. P. Reinhardt, J. Chem. Phys. 59, 4900 (1973).

[23] T. G. Winter and N. F. Lane, Chem. Phys. Lett. 30, 363 (1975).

[24] I. M. Cheshire, Proc. Phys. Soc. (London) 92, 862 (1967).

[25] D. R. Bates, Proc. R. Soc. London Ser. A 247, 194 (1958).

[26] The method was used by Winter, Hatton, and Lane (Refs. 2–5) following the work of Lovell and McElroy [Proc. R. Soc. London Ser. A 283, 100 (1965)] and Winter and Lin [Phys. Rev. A 10, 2141 (1974)] in the context of a bound-atomic-state basis.

[27] E. Merzbacher, *Quantum Mechanics* (Wiley, New York, 1961).

[28] *Handbook of Mathematical Functions,* edited by M. Abramowitz and I. A. Stegun [Natl. Bur. Stand. (U. S.), Applied Mathematics Series 55 (U. S. GPO, Washington, D. C., 1964)].

[29] K. Gottfried, *Quantum Mechanics, Volume I: Fundamentals* (Benjamin, New York, 1966).

[30] S. M. Berman and M. Jacob, Phys. Rev. 139, B1023 (1965).

[31] The equation for $I_{mm'}$ is basically the same as that used in a bound-atomic-state calculation by L. Wilets and D. F. Gallaher [Phys. Rev. A 147, 13 (1966)].

[32] T. G. Winter, Bull. Am. Phys. Soc. 25, 1135 (1980).

[33] B. H. Bransden and C. J. Noble, J. Phys. B 14, 1849 (1981).

[34] D. Rapp, D. Dinwiddie, D. Storm, and T. E. Sharp, Phys. Rev. A 5, 1290 (1972).

[35] There may be numerical inaccuracies in the results of Msezane and Gallaher for the small p-He$^+$ cross section [A. Msezane (private communication)].

[36] B. H. Bransden, C. W. Newby, and C. J. Noble, J. Phys. B 13, 4245 (1980).

[37] W. Fritsch and C. D. Lin (private communication).

[38] B. Peart, R. Grey, and K. T. Dolder, J. Phys. B 10, 2675 (1977).

[39] G. C. Angel, K. F. Dunn, E. C. Sewell, and H. B. Gilbody, J. Phys. B 11, L49 (1978).

[40] G. C. Angel, E. C. Sewell, K. F. Dunn, and H. B. Gilbody, J. Phys. B 11, L297 (1978).

[41] M. B. Shah and H. B. Gilbody, J. Phys. B 11, 121 (1978).

[42] W. L. Nutt, R. W. McCullough, K. Brady, M. B. Shah, and H. B. Gilbody, J. Phys. B 11, 1457 (1978).

[43] J. E. Bayfield and G. A. Khayrallah, Phys. Rev. A 12, 869 (1975).