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Single-electron–removal processes in collisions of positrons and protons with helium at intermediate velocities

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Total cross sections for single ionization and charge transfer have been calculated using the classical-trajectory Monte Carlo (CTMC) technique for collisions of both positrons and protons with helium. Analysis of the classical trajectories has helped to explain the differences in the collision mechanisms responsible for the observed relative magnitudes of the positron and proton electron-removal cross sections. In the intermediate collision velocity range (1.5 a.u. $< v <$ 4.5 a.u.) it is found that because the positron is much smaller in mass than the proton, two dynamical effects occur leading to differences in their efficiency in electron removal. First, positrons are less likely to singly ionize helium than are protons since they possess less kinetic energy above the ionization threshold and accordingly there is a lower probability for ionization. Second, positrons are more likely to remove an electron from helium by charge transfer than are protons since they may be deflected by the target to large positive or negative scattering angles and be accelerated or decelerated to more readily momentum-vector match with an orbital electron. In the large-velocity regime ($v >$ 4.5 a.u.) positrons and protons are found to be equally likely to singly ionize helium, but positrons remain at least half an order of magnitude more likely to remove an electron by charge transfer.

I. INTRODUCTION

Recently, antimatter-atom collisions have attracted an increasing amount of theoretical effort, largely motivated by significant developments made experimentally. The availability of intense low-energy positron beams has only come about in the last few years, leading to a variety of positron and positronium experiments, advances in which have been reviewed by Griffith[1] and by Charlton.[2] One great utility in using antimatter projectiles in collisions with atoms, as illustrated by these and other experiments, lies in the fact that their inclusion in the family of singly charged projectiles $(p,\bar{p},e,\bar{e})$ allows the study of the effects on the reaction when only a single physical parameter is varied, such as the sign of the projectile charge, the projectile mass, or the number of open reaction channels.

For example, analysis by Olson,[3] using the classical-trajectory Monte Carlo (CTMC) method, has explored the effects of the sign of the charge difference between protons and antiprotons in their collisions with helium. That work has helped to identify the collision mechanisms responsible for the unexpectedly large observed[4] ratio of double ionization to single ionization for antiprotons as compared to that for protons. In this related study, we use the CTMC method to elucidate the differences between light (positron) and heavy (proton) -particle mechanisms in single-electron removal collisions with helium, and also compare our results with recent experiments and with other theoretical approaches.

Without using antimatter projectiles to vary the projectile mass, one might consider the difference between electron and proton collisions. However, to do so would be to not only vary the mass but also the sign of the charge and the number of open channels (i.e., for electrons ionization and exchange are possible and for protons, ionization, and charge transfer). Thus, to isolate the mass effect, we compare positron and proton single-electron removal processes, that is, single ionization and single charge transfer,

$$\bar{e}+\mathrm{He} \begin{cases} \to \mathrm{He}^{+}+e+\bar{e}\ , & (1a) \\ \to \mathrm{He}^{+}+\mathrm{Ps}\ , & (1b) \end{cases}$$

$$p+\mathrm{He} \begin{cases} \to \mathrm{He}^{+}+e+p\ , & (2a) \\ \to \mathrm{He}^{+}+\mathrm{H}\ , & (2b) \end{cases}$$

where the sign of the projectile charge and the open reaction channels are the same.

We consider here the intermediate collision velocity range (1.5 a.u. $< v <$ 4.5 a.u.). In this velocity range the CTMC has been demonstrated to be in excellent agreement with experimentally determined total[5] and differential[6] cross sections for heavy-particle–atom electron-removal processes, whereas at higher velocities it underestimates the cross section, primarily due to the lack of inclusion of quantum-mechanical effects. The restriction of the collision velocity to this range is not severe since the experimental measurements for positron-helium scattering made by Fromme *et al.*[7] and by Diana *et al.*,[8] which form the basis for our comparisons, were confined to just this range. The most conspicuous result of these experiments, as they pertain to this work, is that they indicate an enhancement, which increases with velocity, of the cross section for single charge transfer for positrons over that for protons, a trend also indicated by the present calculations.

In the high-velocity regime, Deb, McGuire, and Sil have performed quantum-mechanical calculations of the charge-transfer cross section in proton and positron collisions with hydrogen[9] and helium.[10–12] They find that in this regime (10 a.u. $< v <$ 100 a.u.) second-order processes dominate and that interference effects between the second Born amplitudes account for the enhancement of the positron charge-transfer cross section. Their results and the results of the present work do not agree at the velocity boundary where the two calculations meet, either in the magnitude or the direction of this enhancement trend. These differences are discussed later.

Nonetheless, the present classical study is unique and important in that both the ionization and charge-transfer processes for intermediate velocity positron and protons are treated within a single theoretical framework. Therefore, not only are the effects of the change of a single collision parameter isolated, but the level or type of approximation is also unchanged. In addition, the use of the classical method is valuable because of its ability to illuminate the collision dynamics by allowing examination of the detailed particle trajectories which lead to each class of reaction. Indeed, Deb, McGuire, and Sil have argued[9] that the signature of the second-order processes in electron capture at high velocity is the presence of the Thomas peak, a resonance predicted by a two-step classical model.[13] So, clearly, the use of classical mechanics, while quantitatively useful in its region of validity, may also provide insight for more exact quantum mechanical treatments.

II. THEORETICAL METHOD

Since reactions (1) and (2) involve the removal of only a single electron from helium, we assume that classical contributions from two-electron processes are negligible (i.e., we neglect the target electron-electron interaction). We note, for example, that the double-ionization cross section for proton collisions with helium is 2 orders of magnitude less than the single-ionization value throughout the velocity range studied here.[14] Therefore, we employ a three-body method, the three bodies consisting of the projectile (either a positron or a proton), the target core (He^+), and the active target electron. In reality, the presence of the second target electron increases the probability of single-electron removal even in the absence of the *e-e* interaction simply because there are two electrons, either of which can be removed. To account for this effect, the independent-electron model[15,16] is used to adjust the one-electron transition probabilities calculated for the two independent electron case. These one-electron probabilities are determined by using the three-body, three-dimensional classical-trajectory Monte Carlo method. The form of the CTMC method employed here, which includes all classical forces between the projectile, target core, and active electron, has been described in detail by Percival and Richards,[17] Olson and Salop,[5] and others.

In brief, the CTMC method is a technique in which a large ensemble of projectile-target configurations is sampled in order to simulate the collision process. It consists of three steps: (1) initialization of the projectile-target configuration, (2) calculation of the classical trajectories, and (3) final-state test for reaction. In the first step, the position of the projectile in the plane perpendicular to the incident direction is randomly selected to sample impact-parameter space. Also, according to a classical model of the atom described by Abrines and Percival,[18] the initial orbital eccentricity, orientation, and position of the electron along the orbit are randomly selected. The range of these variables is restricted in such a way that the target ensemble momentum distribution reproduces the quantum-mechanically correct momentum distribution. The accurate reproduction of the target momentum distribution is crucial to the validity of the CTMC approach. To this end, we require that the binding energy match the experimentally determined value for He ($U = -0.904$ a.u. $= -24.6$ eV) and that the radial size of the ensemble of orbits reproduce the dimensions of the actual helium atom which we take as the Hartree-Fock expectation value ($\langle R \rangle = 0.927$ a.u.).[19] From these values we readily define the effective charge that the electron experiences from the hydrogenic model as

$$Z_{\text{eff}} = -2U\langle R \rangle \ , \tag{3}$$

so that $Z_{\text{eff}} = 1.68$.

In the second step, after the initial positions and momenta of all three bodies have been defined, the subsequent motion (classical trajectory) of the particles is found by iteratively solving Hamilton's equations of motion. After the collision, that is, after the integration of the equations of motion has been carried out into the asymptotic region (typically 10 to 20 a.u.), the relative energies of each particle pair (projectile-target core, projectile-electron, and electron-target core) is found to determine what reaction, if any, has occurred during the collision process. This procedure is then repeated until the statistical error (defined below) is sufficiently small. In this work, for each calculation of the total cross section, typically 200 000 trajectories were required to guaranty that the statistical errors were less than 5%.

The total cross section for a particular channel α is determined, in the impact-parameter formulation, as

$$\sigma_\alpha = 2\pi a_0^2 \int_0^{b_{\max}} P_\alpha(b) b \, db \ , \tag{4}$$

where the upper limit of integration $b_{\max}$ is arbitrary, but chosen for efficiency such that the probability $P_\alpha(b)$ is negligibly small for values of the impact parameter b beyond $b_{\max}$. The probability in a particular channel is found in terms of the one-electron probabilities $\tilde{P}_\alpha(b)$ using the independent-electron model. That is, the probability of removing n electrons from a shell containing N electrons is given by

$$P_{\alpha_n}(b) = \begin{bmatrix} N \\ n \end{bmatrix} [\tilde{P}_{\alpha_n}(b)]^n \left[1 - \sum_{\alpha_n} \tilde{P}_{\alpha_n}(b) \right]^{N-n} \ , \tag{5}$$

where the first factor is the binomial coefficient. Thus, for single-electron removal ($n = 1$) from helium ($N = 2$) we have

$$P_{\alpha_1}(b)=2\tilde{P}_{\alpha_1}(b)\left[1-\sum_{\alpha_1}\tilde{P}_{\alpha_1}(b)\right], \quad (6)$$

and specifically, the independent-electron–model single-ionization and single–charge-transfer probabilities become

$$P_{\rm ION}(b)=2\tilde{P}_{\rm ION}(b)[1-\tilde{P}_{\rm ION}(b)-\tilde{P}_{\rm CT}(b)], \quad (7a)$$

$$P_{\rm CT}(b)=2\tilde{P}_{\rm CT}(b)[1-\tilde{P}_{\rm ION}(b)-\tilde{P}_{\rm CT}(b)]. \quad (7b)$$

In the CTMC method, the one-electron probabilities are simply

$$\tilde{P}_{\alpha_1}(b)=N_\alpha(b)/N(b), \quad (8)$$

where $N_\alpha(b)$ is the number of successful final-state tests for channel α and $N(b)$ is the total number of events in any channel. However, since capture to any of the infinity of classically allowed states is possible, we take into account the proper quantum-mechanical density of final states by multiplying the charge-transfer probabilities by the ratio of the final relative momentum to the initial relative momentum, for capture to the ground state. In the case of ionization, because the classical model correctly describes the density of final states (i.e., the continuum), this factor is not appropriate. Thus we have

$$\tilde{P}_{\rm ION}(b)=N_{\rm ION}(b)/N(b), \quad (9a)$$

$$\tilde{P}_{\rm CT}(b)=(k_f/k_i)N_{\rm CT}(b)/N(b). \quad (9b)$$

It is interesting to note that for the positron-helium and proton-helium collision systems in the intermediate velocity regime, the factor in Eqs. (7a) and (7b), namely $2[1-\tilde{P}_{\rm ION}(b)-\tilde{P}_{\rm CT}(b)]$, is only weakly dependent on b and may thus be taken as a constant, depending strongly only on the collision velocity. Therefore we let

$$C(v)=2[1-\tilde{P}_{\rm ION}(b)-\tilde{P}_{\rm CT}(b)]. \quad (10)$$

Using this notation, Eq. (7) may be written as

$$P_\alpha(b)=C(v)\tilde{P}_\alpha(b). \quad (11)$$

This constant, which multiplies the one-electron probabilities, ranges in value between 1 and 2. If it assumed the value of 2, it would indicate that the presence of the second electron in helium would double the one-electron probability for single-electron removal, the maximum that is possible without an *e-e* interaction. On the other hand, a value of 1 would indicate that the second electron had no effect on the single-electron–removal process and this probability would simply be the one-electron result. Typically a value of about 1.6 to 1.8 was found in this work corresponding to a single-electron–removal probability ($\tilde{P}_{\rm ION}+\tilde{P}_{\rm CT}$) in the one-electron approximation of about 10% to 20%.

Also, in practice, only a finite number of impact-parameter bins are used and therefore the integral in Eq. (4) becomes a sum and, using (11), we have

$$\sigma_\alpha=\pi a_0^2 b_{\rm max}^2 C(v)\sum_i N_\alpha(b_i)/N(b_i), \quad (12)$$

or simply

$$\sigma_\alpha=\pi a_0^2 b_{\rm max}^2 C(v)N_\alpha/N, \quad (13)$$

where, for simplicity, the factors k_f/k_i, appropriate to the charge-transfer channel, have been absorbed into the constant $C(v)$. It may be shown that the one standard deviation error limit is given by

$$\Delta\sigma_\alpha=\sigma_\alpha[(N-N_\alpha)/NN_\alpha]^{1/2}. \quad (14)$$

Since in the CTMC method the positions and momenta of each of the particles is known precisely, simple trigonometry yields the pertinent scattering angles and expressions analogous to those for the total cross section and its associated statistical error may be written for the differential cross section. That is,

$$\frac{d\sigma_\alpha}{d\Omega}(\theta)=\pi a_0^2 b_{\rm max}^2 C(v)\frac{N_\alpha(\theta)}{N}\frac{1}{2\pi\sin\theta\, d\theta}, \quad (15)$$

where θ is the scattering angle of the projectile and we use, in effect, an annular detector to maximize the number of counts available so that $d\Omega=\sin\theta\, d\theta$.

At sufficiently small angles the classical model employed here fails to produce the correct form of the differential cross section. In fact, for very small angles, $N_\alpha(\theta)$, the number of counts in the annular detector of size $2\pi\sin\theta\, d\theta$, is roughly constant and therefore, as is evident from Eq. (15), the differential cross section is dominated by the $\sin^{-1}\theta$ behavior and diverges at the origin. To remain finite at very small angles, $N_\alpha(\theta)$ should depend on θ as $\sin\theta$ to cancel the $\sin\theta$ dependence of the solid-angle factor in the denominator. Mason, Vanderslice, and Raw[20] have presented evidence that the classical treatment of the differential cross section is appropriate for angles as small as some critical angle given by

$$\theta_c \simeq \hbar/\mu v b_{\rm max}, \quad (16)$$

where μ is the reduced mass of the projectile-target system, v is the relative collision velocity, and $b_{\rm max}$ approximates the range of the classical interaction. For example, with a collision velocity of 2 a.u. the critical angles for protons and positrons are 0.006 and 9.5 deg, respectively. Therefore, below we present differential cross sections only for angles greater than θ_c.

Despite this incorrect small-angle behavior of the differential cross section, the total cross section is unaffected because it is only the distribution of the counts within the angular range 0 to θ_c deg which is incorrect and not the total number of counts. Thus, the first angular bin of the simulation is chosen to correspond approximately to the range 0 to θ_c deg and integration (summation) of Eq. (15) over all solid angles yields the correct total cross section.

III. RESULTS AND DISCUSSION

In order to find what effect the mass difference between positrons and protons has on single-electron–removal processes in collisions with helium, we have calculated total and differential cross sections for single ionization and single charge transfer. First, we compare these results with experimental measurements to demonstrate the limits of validity of the classical treatment. Then, for both the theoretical and experimental results, we consider the relative magnitudes of the total cross sections for positrons as compared to those for protons, as a function of collision velocity. It should be noted that comparison of the cross sections is made for equal projectile velocities, rather than equal energies, in order to determine the mass dependences. Since it is more common to describe collisions in terms of energy than in terms of velocity, we present in Table I the corresponding positron and proton energies for a few velocities spanning the range of interest. Finally, by analysis of the classical trajectories we propose a model for interpreting the relative magnitudes of the positron and proton cross sections.

A. Proton-impact cross sections

As stated in the Introduction, the calculation of single-electron–removal total[5] and differential[6] cross sections for proton-atom collisions within the CTMC formalism has been demonstrated to yield excellent agreement with experiment in the velocity range of 1 to 4.5 a.u. (25 to 500 keV), a regime in which perturbative treatments have not had as much success. Furthermore, experimental measurements of these proton-impact cross sections have also been made by a number of investigators, with a large degree of agreement among their results. On the other hand, the difficult task of making measurements of the positron-impact processes at comparable collision velocities has only recently been accomplished[7,8] and at least certain aspects of these measurements must be regarded as not well established. Equally less well established is the success of the CTMC method for intermediate velocity light-particle scattering. Thus, in comparing corresponding positron- and proton-impact cross sections, both experimentally and theoretically, it is the proton results which serve as the benchmark.

This fact is demonstrated in part by the excellent agreement between our current CTMC calculations and experimental measurements of the total cross sections for single ionization and for single charge transfer with a helium target as indicated in Figs. 1 and 2, respectively. The experimental data points are taken from Ref. 21 and have been tabulated there from a variety of sources. Therefore, as recommended values, the quoted uncertainty of $\pm 25\%$ is conservative and accounts for the large size of the error bars in these figures.

In the case of ionization by proton impact, Fig. 1, the total cross section reaches its peaks of about 10^{-16} cm^2 at approximately $v=2$ a.u. (100 keV). For $v>2$ a.u. the cross section slowly decreases, the CTMC result showing approximately an E^{-1} dependence, instead of the quantum-mechanically predicted $E^{-1}lnE$ dependence. However, even at $v=4.5$ a.u. (500 keV) the CTMC total cross section is only about 10% low and large discrepancies do not occur except for large velocities, outside the velocity range considered here. For $v<2$ a.u. the behavior of the cross section is due to a competition between ionization and other channels, most importantly, charge transfer (hydrogen formation).

For the proton impacts of very low velocity which succeed in removing an electron, there is a large probability that the electron may become bound, and therefore, charge transfer dominates. For more swift impacts, the proton moves off sufficiently rapidly that the ejected electron is unlikely to become bound, and ionization dominates. This effect accounts for the initial rise in the ionization cross section and the decay from a maximum for charge transfer as velocity increases. The subsequent decay of the ionization cross section is simply due to the fact that the collision time is shortened as the proton velocity increases. The total cross section for charge transfer, displayed in Fig. 2, illustrates this rapid drop off with increasing velocity. In this velocity range, the capture cross section drops by 3 orders of magnitude and obeys approximately an $E^{-3.5}$ dependence. Such behavior has been demonstrated both experimentally and theoretically for atomic hydrogen targets. Thus, below a velocity of about 1.7 a.u. charge transfer dominates, but when the velocity is increased to $v=2$ a.u. the ionization

TABLE I. Positron and proton energies for equivalent velocities.

v (a.u.)	$E_{\bar{e}}$ (eV)	E_p (eV)
1	13.6	25 000
2	54.5	100 000
3	122	225 000
4	218	400 000
5	340	625 000

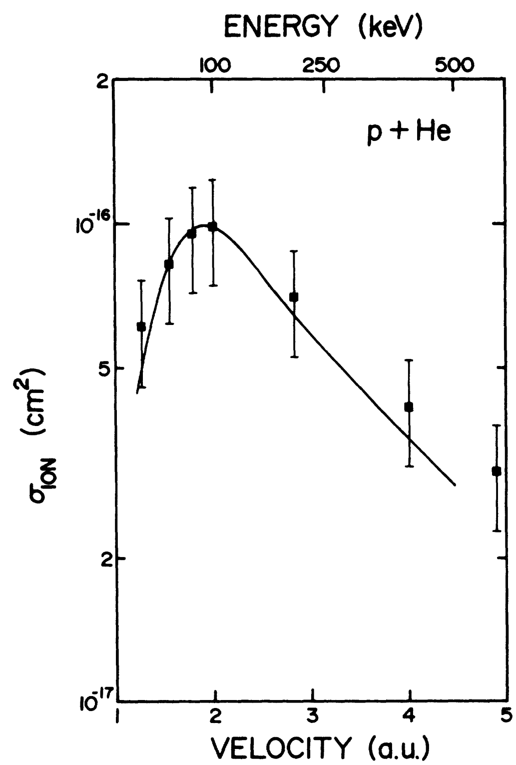

FIG. 1. The total cross section for single ionization of helium by proton impact: CTMC calculation (solid curve), experimental measurements as tabulated in Ref. 21 (closed squares).

cross section is five times that for capture and at $v=4.5$ a.u. the ratio is almost 400.

The differential cross section for single ionization and for single charge transfer for $v=2$ a.u. (100 keV), displayed in Fig. 3, indicates the expected result that proton scattering is very much forward peaked, 90% of the total cross section falling within 0.05 deg (in the laboratory frame) of zero scattering angle. Thus, a proton, whether it removes an electron from the target by ionization or by charge transfer, follows essentially a straight-line trajectory. Included in the figure is the experimental measurements by Martin *et al.*[22] for single charge transfer, illustrating the CTMC method's ability to reproduce angular scattering accurately.

B. Positron-impact cross sections

The total cross section as a function of collision velocity for single ionization of helium by positron impact as determined by our CTMC calculation and by the experiment of Fromme *et al.*[7] is displayed in Fig. 4. The behavior of the cross section is similar to that described for protons above, but an important difference occurs due to the positron's lighter mass. In general terms, at very small velocities ($v<1.7$ a.u.) charge transfer again dominates since the slowly moving positrons readily pick up the knocked-out electrons. As collision velocity increases the ionization process then begins to dominate, as in the proton case, because the positrons tend to be too fast to

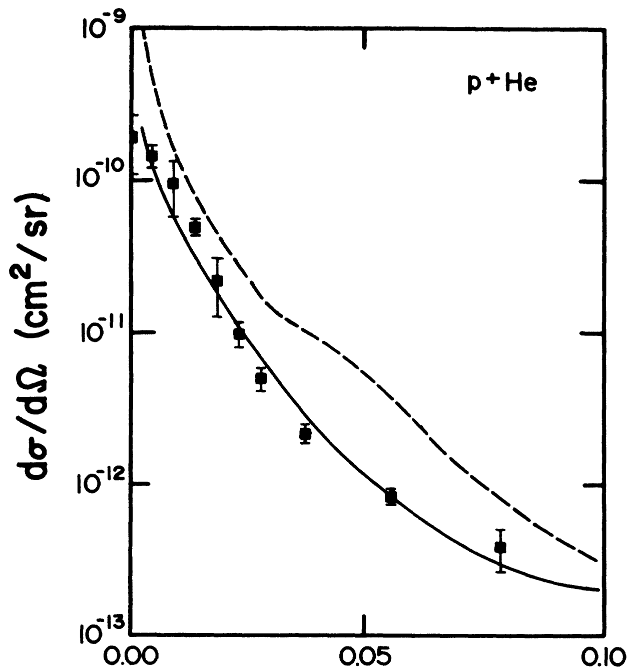

FIG. 3. The differential cross section vs projectile scattering angle for 100 keV ($v=2.0007$ a.u.) protons on helium: CTMC calculation for single ionization (dashed curve), CTMC calculation for single charge transfer (solid curve), and experimental values for single charge transfer measured by Martin *et al.* (Ref. 22) (closed squares).

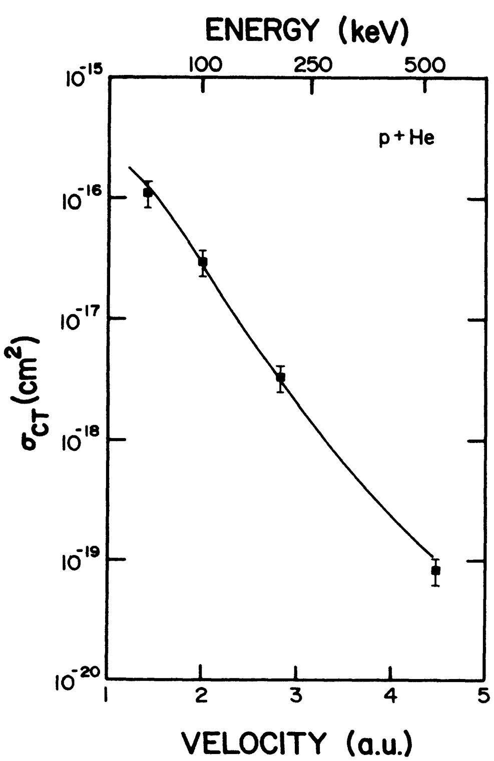

FIG. 2. The total cross sections for single charge transfer in the collision of protons with helium (hydrogen formation): CTMC calculation (solid curve), experimental measurements as tabulated in Ref. 21 (closed squares).

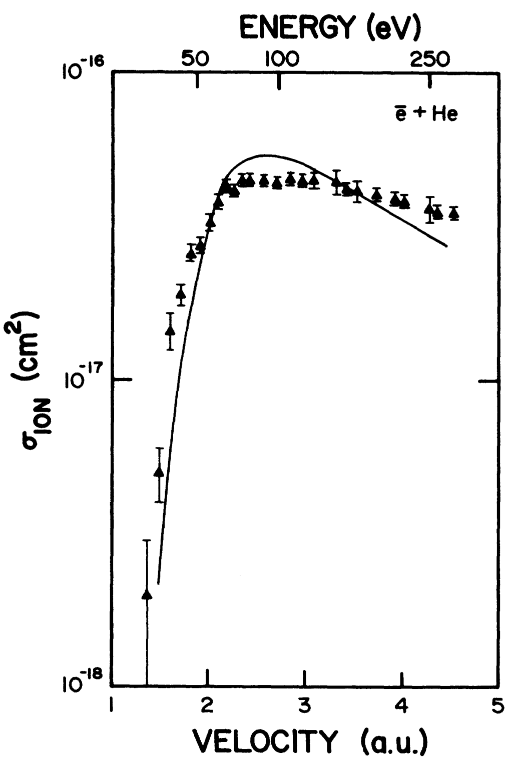

FIG. 4. The total cross section for single ionization of helium by positron impact: CTMC calculation (solid curve), and experimental measurements by Fromme *et al.* (Ref. 7) (closed triangles).

attract the removed electrons. On closer inspection, however, one finds that the low-velocity ($v < 1.7$ a.u.) ionization cross section for positrons is much smaller than for protons. This feature is simply due to the fact that positrons only $\frac{1}{1836}$ the energy of protons at equal velocity and fewer collisions impart sufficient energy to the electron to cause ionization. For example, at $v = 1.7$ a.u. the positron energy is only about 1.6 times the helium first-ionization potential whereas for protons it is about 3000 times the ionization potential. Thus, the ionization curve rapidly rises as the positron energy above ionization threshold becomes substantial.

As compared with the proton total cross section for ionization, the positron total cross section is smaller at low velocities by as much as a factor of 10 (at $v = 1.5$ a.u.) due to this threshold effect. Near the peak around $v = 2$ a.u. the positron cross section is about half the proton cross section and at $v = 4.5$ a.u. the two cross sections are very nearly equal, indicating the diminishing importance of the effect at larger velocities (energies). As in the case of protons, the CTMC method indicates a slightly more rapid fall off for ionization, proportional to E^{-1}, than the experiment predicts (the experimental cross section drops only 25% from $v = 2$ to 4.5 a.u.). For $v < 1.7$ a.u. the CTMC method yields results which are also slightly low. In this velocity range, near threshold, the underestimation of the cross section for ionization arises in large part due to an overestimation of the charge transfer channel.

This overestimation is apparent in Fig. 5 where we plot the CTMC result for single charge transfer along with experimental measurements by Fromme *et al.*[7] and Diana *et al.*[8] Unlike the proton cross section for charge transfer which monotonically falls off in this velocity range, the positron cross section initially rises before decaying. Again this is due to the smaller positron mass and its correspondingly smaller energy above the positronium formation threshold ($E_{\mathrm{Ps}} = 17.6$ eV). In this near-threshold velocity range, the classical model slightly overestimates the charge-transfer process because capture to a continuum of classical atomic states is allowed.

For higher collision velocities ($v > 2$ a.u.) theory and experiment deviate in a more fundamentally important way. The CTMC result indicates that the charge-transfer cross section should fall off as $E^{-3.5}$, a result typical for charged-particle capture. However, the experimental data of Fromme *et al.*[7] indicate a dependence closer to E^{-1} and the data of Diana *et al.*,[8] which have a larger dispersion, show approximately an $E^{-1.5}$ dependence. This difference is also apparent in comparison with other theories. In Fig. 6 we plot the results of the first Born and distorted wave approximations of Mandal, Guha, and Sil,[23] the distorted-wave polarized-orbital method of Khan and Ghosh[24] and the second Born treatment of

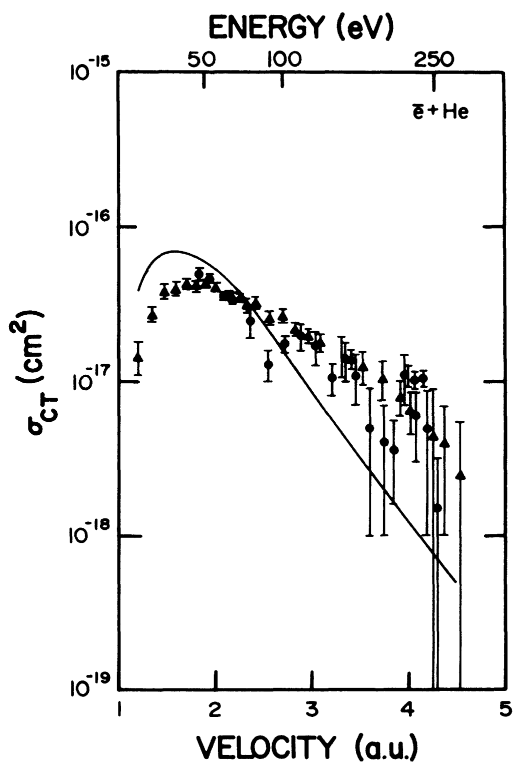

FIG. 5. The total cross section for single charge transfer in the collision of positrons with helium (positronium formation): CTMC calculation (solid curve), experimental measurements by Fromme *et al.* (Ref. 7) (closed triangles), and experimental measurements by Diana *et al.* (Ref. 8) (closed circles).

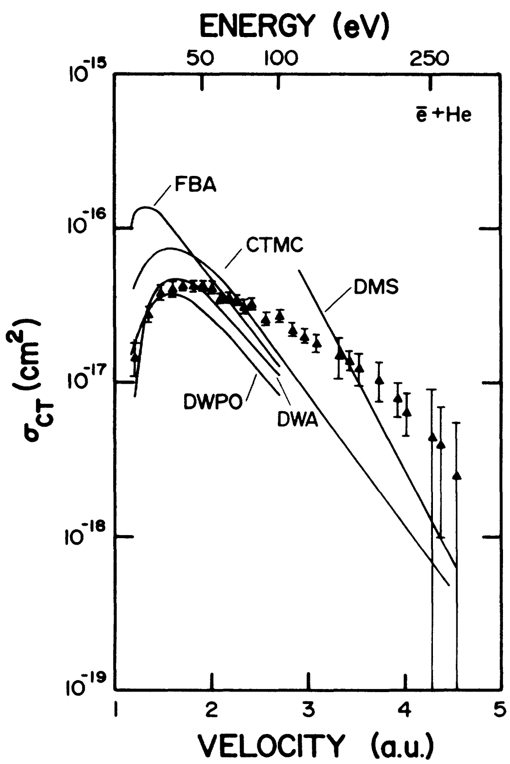

FIG. 6. Comparison between theoretical calculation of the total cross section for single charge transfer in collisions of positrons with helium: (a) first Born approximation (FBA), Mandal, Guha, and Sil (Ref. 23); (b) distorted-wave approximation (DWA), Mandal, Guha, and Sil (Ref. 23); (c) distorted-wave polarized orbital (DWPO) method, Khan and Ghosh (Ref. 24); (d) classical-trajectory Monte Carlo (CTMC) method (present work); (e) Deb-McGuire-Sil second Born approximation (DMS) (Ref. 10); and (f) experimental measurements by Fromme *et al.* (Ref. 7) (closed triangles).

Deb, McGuire, and Sil[10] along with our CTMC calculations and the experimental data of Fromme. Each of these treatments, utilizing a wide variety of techniques and approximations, yields a drop in the cross section proportional to E^{-a} where the exponent falls in the range of $3<a<5$, considerably larger than the experimental result $1<a<1.5$. It should be noted that although the two experimental groups use different methods, neither directly detects positronium in their measurement of the charge-transfer cross sections. The capture cross section is deduced from a difference in observable values.

However, we suggest that this discrepancy between theory and experiment may be explained as follows. Each of the experiments rely on a solenoidal magnetic field to confine the positron beam to the forward direction as it passes through the target gas region. Positrons which are removed from the beam are then inferred to have formed positronium. If, however, the scattering of positrons in the ionization process proceeds to large angles, then for large collision velocities, there should be some angle $\gamma(v)$, for which the transverse velocity is great enough to prohibit confinement. By evaluating the fraction of the total cross section within various angular regimes, (see Table II), we find that significant large angle scattering persists to relatively large collision velocities. Therefore, there would be a loss of flux attributed to charge transfer which actually results from large angle scattering processes such as ionization. The measured cross section for charge transfer would then be

$$\sigma'_{\mathrm{CT}}=\sigma_{\mathrm{CT}}+f(v)\sigma_{\mathrm{ION}}\ , \tag{17}$$

where f is the fraction defined by

$$f(v)=\sigma_{\mathrm{ION}}[\theta>\gamma(v)]/\sigma_{\mathrm{ION}}(v)\ . \tag{18}$$

Clearly, $\gamma(v)$ depends on velocity since for small velocities the magnetic field is strong enough to bend even the positrons scattered to large angles back into the forward direction, but as velocity increases these large-angle scattered positrons become too fast to confine. This velocity dependence explains why the discrepancy occurs for velocities above 3 a.u., at smaller velocities $f(v)$ being about zero.

To see if this prediction is reasonable we have assumed that above $v=3$ a.u. $\gamma=45$ deg and then used the CTMC results in Eq. (17). For example, at $v=3.8$ a.u. we find that $f=0.19$ and we deduce an observed value of $\sigma'_{\mathrm{CT}}=8.5\times10^{-18}$ cm^2 (the experimental value being 9.2×10^{-18} cm^2) and at $v=4.5$ a.u. we find that $f=0.12$ and $\sigma'_{\mathrm{CT}}=3.9\times10^{-18}$ cm^2 (the experimental value being 3.1×10^{-18} cm^2). Thus, by accounting for the loss of flux to large scattering angle ionizations, the experimental behavior can be reproduced.

In fact, since for large velocities σ_{ION} is much larger than σ_{CT}, the measured cross section should behave as

$$\sigma'_{\mathrm{CT}}\sim f(v)\sigma_{\mathrm{ION}}(v)\ . \tag{19}$$

Also, we find that the fraction not confined is inversely proportional to velocity and since the ionization cross section decreases approximately as E^{-1} we have

$$\sigma'_{\mathrm{CT}}\sim v^{-1}E^{-1}\ , \tag{20}$$

which is the $E^{-1.5}$ behavior observed.

Further observation of the rate of decline of the charge-transfer cross section with increasing velocity seems in order, as well as further theoretical investigation. Partly to this aim, and partly to illustrate the non-straight-line trajectory nature of the positron-impact processes, we have calculated cross sections differential in the projectile angle for several velocities. These differential cross sections are displayed in Figs. 7 and 8. Also in Table II we have tabulated the laboratory acceptance angles required to obtain various percentages of the total cross section. As the graphs and the table indicate for both ionization and charge transfer, the positron may be deflected to large angles in its collision with helium. Figures 7 and 8 also reflect the changing dominance of the capture and ionization processes as the collision velocity is raised from $v=2$ to 3.8 a.u. It should be noted that the CTMC method does not predict an observable Thomas scattering peak at 45 deg at intermediate velocities.

C. Ratios

In Figs. 9, 10, and 11 we compare the single-electron–removal mechanisms in positron-helium and

TABLE II. CTMC laboratory acceptance angles (scattering angle range 0 to θ deg) required to observe various percentages of the total cross section.

Process	Velocity (a.u.)	θ (10%) (deg)	θ (50%) (deg)	θ (90%) (deg)
1-CT ($\bar{e}+$He)	2	3.7	18.6	46.0
1-ION ($\bar{e}+$He)	2	6.3	26.7	67.9
1-CT ($p+$He)	2	<0.003	0.014	0.049
1-ION($p+$He)	2	<0.003	0.012	0.051
1-CT ($\bar{e}+$He)	3.8	4.7	16.8	40.8
1-ION ($\bar{e}+$He)	3.8	3.6	17.7	48.7
1-CTC ($p+$He)	3.8	0.003	0.006	0.0045
1-ION ($p+$He)	3.8	<0.003	0.007	0.025

proton-helium collisions by plotting the ratios of the positron and proton cross sections as a function of collision velocity. By comparing projectiles of equal velocity, this procedure helps to illuminate the differences caused by varying the mass of the projectile. Additional insight into the collision mechanisms may be drawn by detailed observation of individual trajectories which lead to electron removal. Since we employ the CTMC method, this examination of particle trajectories is easily accomplished by displaying them graphically on a computer terminal, resulting in a "movie" of each collision selected from the ensemble. From these procedures a simple model of the positron and proton single-electron-removal process may be proposed.

For example, in Fig. 9 we display the ratio of the positron and proton single-ionization cross sections. For small collision velocities, protons are much more efficient at ionizing helium because of a simple kinematical effect, that is, because of the positron's smaller mass and accordingly smaller energy above-ionization threshold, fewer collisions lead to ionization. In fact, at $v = 1.35$ a.u. the positron energy is less than half an eV above threshold whereas the proton energy is about 45.5 keV above threshold. However, for large velocities the energy difference rapidly diminishes in importance to the ionization mechanism since the positron's energy is sufficiently far above the threshold. Our CTMC results, as well as the experimental measurements, indicate that once the positron energy has reached about ten times the ioniza-

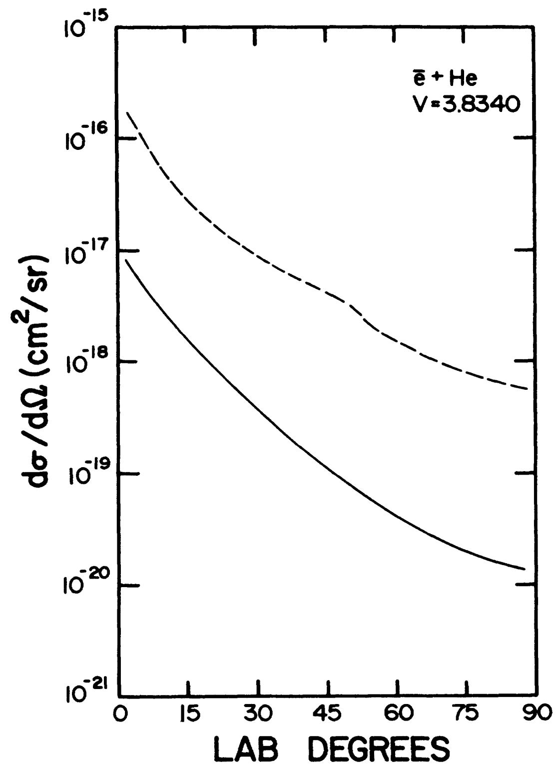

FIG. 8. Same as Fig. 7 except for 200 eV ($v = 3.8340$ a.u.) positrons on helium.

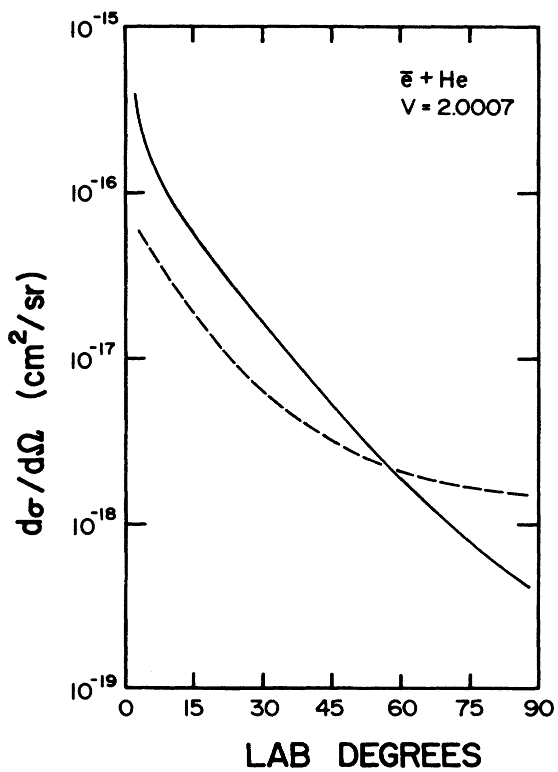

FIG. 7. The differential cross section vs projectile scattering angle for 54.5 eV ($v = 2.0007$ a.u.) positrons on helium: CTMC calculation for single ionization (dashed curve), CTMC calculation for single charge transfer (solid curve).

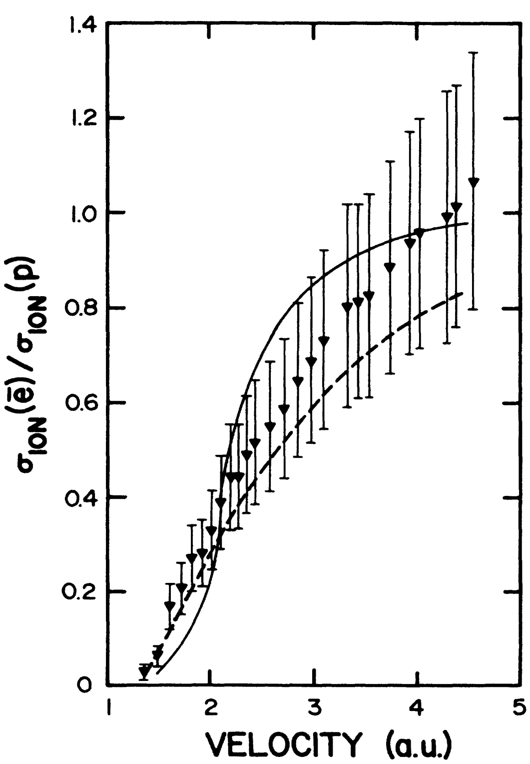

FIG. 9. Ratio of the total cross section for single ionization of helium by positron impact to that by proton impact: CTMC calculation (solid curve) and experimental points (inverted triangles) are the ratio of the measurements by Fromme *et al.* for positrons to those tabulated in Ref. 21 for proton impact. Ratio of electron impact ionization to proton-impact ionization: experimental points (dashed curve) from Ref. 21.

tion threshold ($v > 4.25$ a.u.) the positron and proton cross sections will be approximately equal in magnitude. Thus, asymptotically the ratio for ionization becomes one.

Further evidence that the difference between the positron- and proton-impact ionization cross sections results only from the difference in energy comes from examining the ratio of the electron- and proton-impact ionization cross sections. This ratio is included in Fig. 9 as a dashed line and is a rough fit to tabulated experimental data.[21] Clearly, the electron-to-proton ionization ratio indicates the same general behavior as the positron-to-proton ratio. In this case too, since the lighter particle has little energy above threshold fewer collisions result in ionization at small velocities. As the energy above threshold increases, however, it also becomes equally as likely to ionize the target as the heavier particle. The difference in the cross sections for the two light particles, positrons, and electrons, reflects the difference in the sign of their charge. This results in branching between different open scattering channels (i.e., positron: ionization and charge transfer; electron: ionization and exchange) and a difference in the electron removal mechanism (i.e., positron: attraction; electron: repulsion).

The ratio for single charge transfer, displayed in Fig. 10, indicates that at small velocities ($v < 2$ a.u.) positrons are less likely to remove an electron from helium by capture than are protons of equal velocity. As in the case of ionization, the positrons have little energy above the capture threshold and accordingly fewer collisions lead to charge transfer. Also as in the ionization case, this effect diminishes as velocity increases. Unlike the ratio for ionization which goes to one in the limit of large velocities, for velocities above 2 a.u. the ratio for charge transfer becomes greater than one. This fact is borne out by both experiment and theory. The present CTMC calculations indicate that positrons are more likely to capture an electron than are protons by about a factor of 5 at large velocities ($v > 4$ a.u.), however, experiment indicates that the ratio may be much larger.

Since the proton charge-transfer cross section is well established both experimentally and theoretically (see Fig. 2) it is the lack of agreement between experiment and theory on the positron charge-transfer cross section which accounts for this disagreement in the ratio at velocities greater than about 3 a.u. In particular, it is the rate of decrease of the positron cross section as a function of energy that differs between theory and experiment. As discussed above, there is general agreement between theories that the rate of decrease should be proportional to about E^{-4} whereas the experiments indicate approximately an E^{-1} dependence. Thus, for $v > 3$ a.u. the experimental cross section is larger than theoretically predicted and, consequently, the positron-to-proton ratio is larger as well. Therefore, the correct value of the ratio for charge transfer is critically dependent on resolving

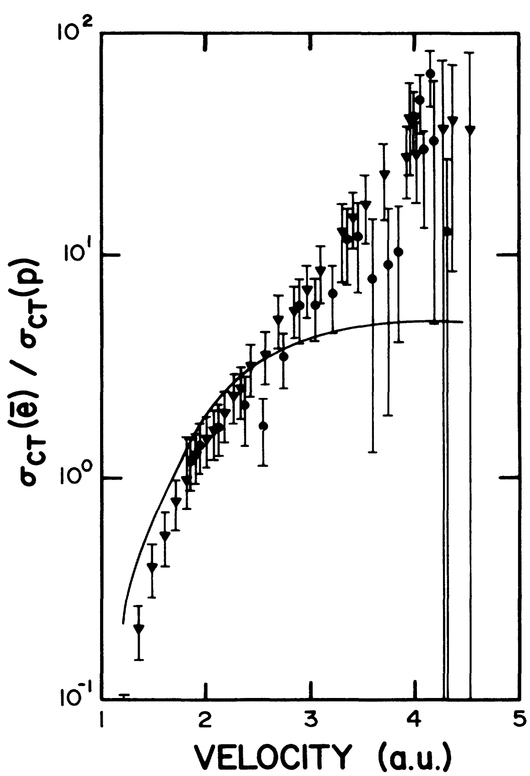

FIG. 10. Ratio of the total cross section for single charge transfer in collisions between positrons and helium to that for collisions between protons and helium (ratio of positronium formation to hydrogen formation): symbols are the same as in Fig. 10 with the addition of experimental points (full circles) which are the ratio of the measurements by Diana *et al.* for positron impact to those tabulated in Ref. 21 for proton impact.

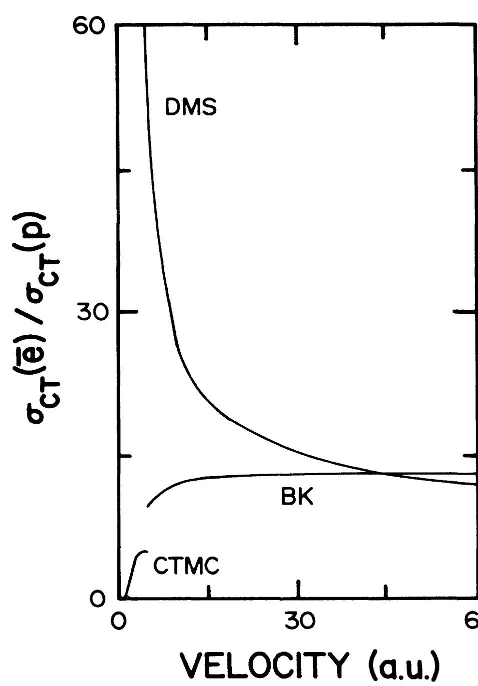

FIG. 11. Comparison between theoretical calculations of the ratio of the total cross section for single charge transfer in collisions between positrons and helium to that for collisions between protons and helium: (a) Deb-McGuire-Sil second Born approximation (DMS) (Ref. 10); (b) Brinkman-Kramer approximation (Ref. 10); and (c) CTMC (present work).

the disagreement at velocities greater than about 3 a.u. where we have proposed a possible cause due to large-angle scattering in the ionization channel. Nevertheless, a sensible picture of why the ratio for capture is asymptotically greater than 1 may still be drawn.

The basis for this picture is the fact that positrons are lighter than protons and therefore possess smaller momenta. One obvious consequence is that positrons may more easily be scattered to large positive or negative angles while proton trajectories remain substantially undeflected. This behavior is reflected in the scattering-angle differential cross sections presented above. For example, a laboratory acceptance angle of only 0.05 deg is required to observe 90% of the total cross section for charge transfer for protons of velocity 2 a.u. Positrons of equal velocity require an acceptance angle of about 46 deg to observe a similar percentage of the total cross section (see Table II). The partitioning between positive and negative scattering angles, that is whether the projectile is deflected away or towards the helium atom, depends primarily on the impact parameter. While easily discernable with the CTMC method, this partitioning might be experimentally accessible by observing the ion recoil momentum.

Another consequence of the positron's smaller momenta is that its speed may be more readily changed. In fact, in the collision complex (i.e., the pseudomolecule formed temporarily at the time of the collision) the positron may be either accelerated or decelerated by the target before capturing an electron. Of course, after the charge-transfer collision the positronium formed moves off with a smaller velocity than the incident positron, since in the capture process the positron must share its kinetic energy equally with the electron. Protons, on the other hand, suffer very little change in their velocity in the capture process and the hydrogen atom formed moves off at essentially the same speed as the incident proton.

These observations lead to the following model for the capture process. Because of the large mass and momentum of the proton, the atomic electron must have a position and momentum which allows it to easily "jump onto" the proton as it passes by. In the process, the proton remains mostly undeflected and is not slowed down. Obviously, as the proton's velocity increases, the electron finds it more difficult to transfer and the cross section for hydrogen formation decreases. In the positron impact case, because of its small mass and momentum, the positron may be substantially deflected (in a direction toward or away from the nucleus) and have its speed decreased or even temporarily increased so that it may effectively vector-momentum match with an orbital electron. The result is a positron-electron pair that tumbles off (i.e., the positron and electron rotate about their center of mass) at possibly large angles. Thus, once the positron velocity is sufficiently great that the positronium formation threshold is no longer significant, its ability to momentum-vector match with an orbital electron causes it to be more likely to capture an electron than a proton of equal velocity.

An interesting way of looking at this effect is in terms of the available phase space for the reaction. Since the proton follows a straight line and is not slowed down in the collision, and the positron may be deflected to large positive or negative angles and may be slowed or temporarily sped up to varying degrees, the phase space available for the capture by protons is smaller than that for positrons. A method of calculating the phase-space volumes in collisions of the type $A+BC \rightarrow AB+C$ for the case of atom-diatom collisions has been developed by Light.[25] A simplified version of this technique might yield insight into the relative magnitudes of the positron and proton cross sections by considering the analog collision in which the projectile positron or proton (A) collides with a helium target composed of a core (B) plus an active electron (C). Using this method, the ratio of the positron and proton cross sections for charge transfer would be

$$\frac{\sigma_{\rm CT}(\bar{e}+{\rm He})}{\sigma_{\rm CT}(p+{\rm He})}=\frac{\Gamma_{\rm CT}(\bar{e}+{\rm He})\Big/\sum_i \Gamma_i(\bar{e}+{\rm He})}{\Gamma_{\rm CT}(p+{\rm He})\Big/\sum_i \Gamma_i(p+{\rm He})} ,$$

where Γ_i denotes the volume in phase space for a particular channel and the summations represent the total phase space available for any channel consistent with conservation of energy and momentum. This may be of more than just academic interest because it might shed further light on the value of the exponent in the decay of the charge-transfer cross section as a function of energy for positrons, using a fundamentally different approach to calculate the ratio.

It seems clear, by comparison with experiment, that in the velocity regime considered here, the CTMC method reproduces the correct trends in the ratios for both ionization and charge transfer. Also, in the limit of large velocities, it seems reasonable to predict that positrons and protons are equally likely to singly ionize helium and that positrons should remain more likely to remove an electron by capture than protons of equal velocity. However, since the classical method is not valid at velocities much above $v=4.5$ a.u., and since no positronium formation measurements exist for higher velocities, there remains some question as to the value for the charge-transfer ratio asymptotically. In Fig. 11 we compare our results with those of Deb, McGuire, and Sil[10] who have used second Born treatments of the positron and proton charge-transfer collisions with helium. Also displayed with these calculations, which are expected to be valid at large velocities, is the Brinkman-Kramers approximation.

Taken alone, this figure indicates that the CTMC and Brinkman-Kramers approximation are in rough agreement, they predict that the capture ratio should rise sharply initially, as velocity is increased and the threshold effect becomes negligible, and asymptotically level off at value of about ten. It is clear that charge transfer measurements for higher velocity positron-helium collisions would be desirable as well as further investigation of the experimental rate of decay as a function of energy in the present regime.

IV. SUMMARY

Using the CTMC method we have calculated total and differential cross sections for single-ionization and single–charge-transfer for positron- and proton-helium collisions. In the velocity range 1.5 a.u. $< v <$ 4.5 a.u. excellent agreement between theory and experiment has been demonstrated for proton-helium collisions leading to single-electron removal. Also in this velocity range, reasonable agreement with recent experimental determinations of the positron-helium cross sections has been obtained, the most significant deviation occurring in the charge-transfer cross section at velocities greater than 3 a.u. In this case our CTMC results indicate that the cross section should fall off as $E^{-3.5}$, approximately as do other theoretical approaches, whereas experiment indicates approximately an E^{-1} dependence. We suggest that this discrepancy arises from experimentally unexpected large angle positron scattering in the ionization channel.

Also, by examining the ratio of the positron-impact cross sections to those for proton impact at equal velocities, as well as by detailed examination of individual classical trajectories, a model has been suggested to explain the relative efficiencies of positrons and protons at single-electron removal resulting from their mass difference. The initial rise as a function of velocity in these ratios stems from the positron's gain of sufficient energy above the reaction (ionization or charge transfer) threshold. In the limit of large velocities, positrons should be equally likely to singly ionize helium as protons of equal velocity. Also, asymptotically, positrons should become at least five times as likely to capture an electron from helium as protons of equal velocity due to their ability to momentum-vector match more readily with an orbital electron.

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