Stripping of μ^- from $\alpha\mu$ after muon-catalyzed fusion: Effect of target structure

James S. Cohen
Theoretical Division, Los Alamos National Laboratory, University of California, Los Alamos, New Mexico 87545
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Stripping (ionization and transfer) and excitation cross sections for the muonic helium ion ($\alpha\mu$) in deuterium-tritium mixtures are calculated by the classical-trajectory Monte Carlo method. It is shown by direct (three- and four-body) calculations that the effects of the target electronic structure and finite mass are not important.

I. INTRODUCTION

When the mesomolecular ion $dt\mu$ is formed following muon stopping in a high-density deuterium-tritium mixture, nuclear fusion rapidly ensues.[1] After the fusion the muon is either left free to catalyze another fusion or "sticks" to the positively charged fusion product,

$$dt\mu \rightarrow \begin{cases} n+\alpha+\mu & \text{(1a)} \\ n+\alpha\mu & \text{(1b)} \end{cases} .$$

In the latter event the muon is lost from the catalysis cycle unless it is freed in a collision, e.g.,

$$\alpha\mu+d \rightarrow \begin{cases} \alpha+\mu+d & \text{(2a)} \\ \alpha+d\mu & \text{(2b)} \end{cases} ,$$

before the $\alpha\mu$ is slowed from its initial velocity of 5.83 a.u. to a velocity less than 1 a.u.[2] Previous calculations have found this reactivation probability[3,4] to be $\sim 24\%$, which when combined with the recently calculated branching ratio[5,6] of $\sim 0.9\%$ for (1b) predicts an effective "sticking" probability of $\sim 0.7\%$.

Recent experiments,[7] however, have shown that the sticking probability is smaller than the above value, 0.35% at liquid-hydrogen density, and, furthermore, depends on the target density.[8] It should be noted that both the slowing-down (stopping) and stripping rates for reactions (2) depend linearly on density, so no density dependence of the stripping probability can be obtained from the simplest possible description based on the competition between these two processes. The most likely source of a net density dependence would appear to be radiative processes,[3] which are independent of the density and important in $(\alpha\mu)_n$ deexcitation at low n (n is the principal quantum number). The ionization and charge-transfer cross sections depend strongly on the state of $\alpha\mu$. However, calculations based on existing cross sections find that the excited-state populations are relatively small and predict a variation of the sticking probability over an order of magnitude less than that observed.[9,10]

All previous theoretical determinations of stripping cross sections ignore the electronic structure of the target. This would appear to be a reasonable approximation, at least at high velocities, owing to the muon- to electron-mass ratio of ~ 207; nevertheless, in view of the discrepancy with experiment and speculations on its explanation, the present calculations were undertaken in part to determine the effect of finite target mass and electronic structure on the $\alpha\mu$ stripping (ionization and charge transfer) and excitation. As will be seen, the effect of atomic structure is found to be so small that it is considered unnecessary to treat explicitly the additional structure of the actual molecular target. The classical-trajectory Monte Carlo (CTMC) method is used and is expected to be reliable for collisions at moderate velocities. This method has been used previously for ionization and charge transfer in collisions of $\alpha\mu$ with bare protons[3]—the present calculations reduce the statistical error bars on these cross sections.

Of particular interest is the effect of the target electron

TABLE I. Results (see Ref. 2) of three-body CTMC $\alpha\mu+d$ calculations for $\alpha\mu$ initially in its ground state.

v	σ_1^{ion}	σ_1^{tr}	σ_1^{st}	σ_{12}	σ_{13}	$\sigma_{1,\geq 4}$
1	0.009	0.95	0.96	0.18	0.009	0.006
2[a]	0.36	0.74	1.10	0.30	0.06	0.06
3	0.50	0.13	0.63	0.36	0.06	0.05
4	0.31	0.019	0.33	0.28	0.05	0.03
5	0.22	0.003	0.22	0.18	0.03	0.02
6[a]	0.148	0.0008	0.149	0.161	0.020	0.016
12[b]	0.038		0.038	0.052	0.006	0.005
18[b]	0.0162		0.0162	0.0212	0.0028	0.0016

[a]Additional trajectories were run at $v=2$ and $v=6$ to reduce the standard deviation of σ_1^{st} to 2%.
[b]The Born approximation may be expected to be better than the classical approximation at these high velocities. The CTMC results are presented here for comparison to excited states via the classical scaling law and for verification of the classical $1/v^2$ high-energy behavior.

on cross sections for collisions of excited state $\alpha\mu$. For the three-body collision $(\alpha\mu)_n + d$, a simple classical scaling law[11] gives the cross section for $n > 1$ in terms of the cross section for $n = 1$ at a different energy. However, this scaling law is not strictly applicable when the $1s$ electron is bound to the deuteron. If stripping cross sections for excited states were increased, the effect would be to enhance the density dependence of the sticking probability.

II. THEORETICAL METHOD

The CTMC method was applied in three ways: (1) collision of $\alpha\mu$ with a bare nucleus, p, d, or t; (2) collision of $\alpha\mu$ with an "atom" represented by a *static* effective potential (still a three-body calculation); and (3) collision of $\alpha\mu$ with an atom D ("de" following our alternate notation) in which the electron dynamics is also treated classically (a four-body calculation). The calculations of type 1 were performed as a standard for comparison; the potential in this case is simply the sum of three pure Coulomb potentials. In the calculations of type 2 the atom is represented with an r-dependent effective charge,[12] $(1+r)\exp(-2r)$, and will be denoted D_{eff}. This treatment approximately takes care of one effect of the target electron, namely, shielding of the nuclear charge, and has the advantage of utilizing the quantum-mechanical electron density. Calculations of type 3 were done to determine, in addition, the effect of direct collisions with the finite-mass electron.

Four-body calculations of chemical dynamics have previously been made, and the dynamical equations for four-body ion-atom collisions are completely analogous. The center-of-mass motion was separated using the AB + CD coordinate system described by Raff *et al.*,[13] and the resulting system of 18 Hamilton equations were integrated numerically. The initial conditions of both the $\alpha\mu$ and de atoms were chosen from microcanonical distributions.[14] Hence the muon and electron are initially bound by the actual ionization potentials. These distributions are spherically symmetric and so represent a statistical combination of the various l values that are possible in excited states—this averaging is generally appropriate since the l-mixing cross sections are large.[15]

The statistical error of the Monte Carlo calculations decreases only as the inverse of the square root of the number of reactive trajectories. This makes comparison of results obtained under slightly different conditions difficult if the statistics of different runs are completely uncorrelated. To facilitate such comparisons, the runs of types 1, 2, and 3 were made using the *same* initial conditions insofar as possible. In the case of type-3 calculations, the c.m.$(\alpha\mu)$−c.m.(de) coordinates were made the same as the c.m.$(\alpha\mu)-d$ coordinates in type-1 and -2 calculations. This procedure is designed to make the *relative* precisions better than the standard deviation of individual results.

III. RESULTS

The following calculations were performed:

(1) $(\alpha\mu)_n + d$ for $v = 1$, 2, 3, 4, 5, 6, 12, and 18 a.u. and

TABLE II. Results of three- and four-body CTMC $\alpha\mu + D$ calculations for $\alpha\mu$ initially in spherically symmetric states with $n = 1$, 2, and 3. Results are given for the bare nuclear (d) target and static (D_{eff}) and dynamic (de) neutral atomic targets. One standard deviation of σ_n^{st} is 5% in all cases.

Target	σ_1^{ion}	σ_1^{tr}	σ_1^{st}	σ_{12}	σ_{13}	$\sigma_{1,\geq 4}$	σ_2^{ion}	σ_2^{tr}	σ_2^{st}	σ_{23}	$\sigma_{2,\geq 4}$	σ_3^{ion}	σ_3^{tr}	σ_3^{st}	$\sigma_{3,\geq 4}$
(a) $v = 1$ a.u.															
d	0.009	0.96	0.96	0.177	0.009	0.006	5.7	11.7	17.4	8.1	4.7	40	11.4	51	103
D_{eff}	0.009	0.96	0.96	0.181	0.006	0.012	6.0	11.7	17.6	8.2	4.5	40	11.2	51	105
de	0.009	0.89	0.90	0.201	0.015	0.005	5.7	11.7	17.4	8.3	4.7	40	11.4	51	103
(b) $v = 6$ a.u.															
d	0.144	0.0003	0.145	0.178	0.026	0.013	0.60		0.60	1.72	0.47	1.30		1.30	9.8
D_{eff}	0.144	0.0003	0.145	0.178	0.026	0.013	0.60		0.60	1.72	0.47	1.30		1.30	9.8
de	0.145	0.0003	0.146	0.161	0.022	0.017	0.59		0.59	1.75	0.49	1.33		1.33	9.7

TABLE III. Results of three-body CTMC calculations for $\alpha\mu$ collisions with p, d, and t. For $v=2$ a.u. additional sets of trajectories were run to estimate the uncertainty in the isotope dependence, designated d/p and t/d.

Target	σ_1^{ion}	σ_1^{tr}	σ_1^{st}	σ_{12}	σ_{13}	$\sigma_{1,\geq 4}$
			(a) $v=2$ a.u.			
p	0.33	0.73	1.06	0.30	0.05	0.05
d	0.36	0.74	1.10	0.30	0.06	0.06
t	0.38	0.74	1.12	0.30	0.06	0.05
d/p	1.08±0.04	1.02±0.01	1.04±0.01	1.02±0.02	1.04±0.11	1.12±0.16
t/d	1.06±0.01	1.00±0.01	1.02±0.01	1.00±0.01	1.00±0.06	0.92±0.08
			(b) $v=6$ a.u.			
p	0.144	0.0006	0.145	0.176	0.029	0.012
d	0.144	0.0003	0.145	0.178	0.026	0.013
t	0.144		0.144	0.176	0.027	0.013

$n=1$;

(2) $(\alpha\mu)_n+d$, $(\alpha\mu)_n+D_{\text{eff}}$, and $(\alpha\mu)_n+de$ for $v=1$ and 6 a.u. and $n=1$, 2, and 3;

(3) $(\alpha\mu)_n+p$ and $(\alpha\mu)_n+t$ for $v=2$ and 6 a.u. and $n=1$.

The results are given in Tables I–III. Enough trajectories were run that the standard deviation of every total-stripping cross section σ_n^{st} was reduced to 5%. The uncertainties in other cross sections for the same collision are given approximately by

$$\Delta\sigma_{\text{other}}\approx(\sigma_{\text{other}}/\sigma_n^{\text{st}})^{1/2}\Delta\sigma_n^{\text{st}} , \tag{3}$$

which for the precision of the present calculations implies the relative error

$$\frac{\Delta\sigma_{\text{other}}}{\sigma_{\text{other}}}\approx 0.05\left[\frac{\sigma_n^{\text{st}}}{\sigma_{\text{other}}}\right]^{1/2} .$$

The other cross sections tabulated are the two components of stripping (the ionization cross section σ_n^{ion} and the muon-transfer cross section σ_n^{tr}) and the excitation cross sections $\sigma_{n,n'}$.

The CTMC treatment of the inelastic cross sections is not as satisfactory as the treatment of stripping. Excitation and deexcitation are not treated symmetrically; i.e., the initial energy is taken to be precisely the quantum value, but the final-state binding energy must be placed in bins.[16] This ambiguity is most serious for deexcitation into low n, and it is probably more reliable to obtain the inelastic deexcitation cross sections from the corresponding excitation cross sections by the detailed balance relationship.

As can be seen in Table I, stripping is mainly due to transfer at $v\lesssim 2$ and to ionization at $v\gtrsim 3$. At high velocities it is well known that the classical ionization cross section falls off as $1/v^2$, whereas the quantum-mechanical dependence is $(\ln v)/v^2$; this failing must be taken into account for $v>6$. Nevertheless, the classical results given in Table I for $v>6$ are of interest because of the classical scaling law relating the cross section for $n=1$ to cross sections for $n\geq 2$, for which the classical treatment is good.[17] At $v\gtrsim 6$,

$$\sigma_1^{\text{ion}}\approx 5.3/v^2 . \tag{4}$$

The classical scaling law for the Coulomb potential is

$$\sigma_n(v)=n^4\sigma_1(nv) . \tag{5}$$

Combining Eqs. (4) and (5) yields

$$\sigma_n^{\text{ion}}(v)\approx 5.3n^2/v^2 , \tag{6}$$

which is expected to be very good for $n\geq 2$. This relation can be numerically verified by the first line in Table II(b).

The CTMC results are in good agreement with results of the Born approximation[3] for σ_1^{ion}, σ_{12}, and σ_{13} at $v\sim 6$. However, at lower velocities the CTMC cross sections are smaller than the Born values, suggesting that the Born approximation is not adequate at $v\lesssim 3$ a.u.

The results discussed so far have neglected the electronic structure of the target. It is clear from Table II that the effect of the electron, whether treated statically or dynamically, is very small and certainly no greater than the uncertainty in the present calculations. We have shown that neither the shielding of the nuclear charge by the electron nor collisions with the electron is of importance in $\alpha\mu$ collisions at velocities $\gtrsim 1$ a.u. Hence the scaling law (5) is still quite appropriate even though the fixed (unscaled) energy of the target electron invalidates it in principle. Furthermore, the results in Table III show that the effect of the finite target mass is also small and is negligible at velocities as high as 6 a.u. We conclude that in calculations of stripping of $\alpha\mu$ in deuterium-tritium mixtures, it is an excellent approximation to neglect the electronic (including molecular[18]) structure and a fairly good approximation to neglect the isotope dependence. The electronic and isotopic effects on muon stripping are too small to be observed in current muon-catalyzed-fusion experiments.

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[1]L. Bracci and G. Fiorentini, Phys. Rep. **86**, 169 (1982).
[2]Muonic atomic units, $\hbar = e = m_\mu = 1$, are used except where otherwise stated. The unit of velocity is equal to 2.19×10^8 cm/s and the unit cross section is 6.55×10^{-22} cm^2.
[3]L. Bracci and G. Fiorentini, Nucl. Phys. **A364**, 383 (1981).
[4]S. S. Gershtein *et al.*, Zh. Eksp. Teor. Fiz. **80**, 1690 (1981) [Sov. Phys.—JETP **53**, 872 (1981)].
[5]D. Ceperley and B. J. Alder, Phys. Rev. A **31**, 1999 (1985).
[6]C.-Y. Hu, Phys. Rev. A **34**, 2536 (1986); L. N. Bogdanova *et al.*, Nucl. Phys. **A454**, 653 (1986).
[7]S. E. Jones *et al.*, Phys. Rev. Lett. **56**, 588 (1986).
[8]Preliminary analysis of the data also suggested some dependence on the tritium fraction, but the complete analysis indicated that that dependence was not statistically significant.
[9]L. I. Men'shikov and L. I. Ponomarev, Pis'ma Zh. Eksp. Teor. Fiz. **41**, 511 (1985) [JETP Lett. **41**, 623 (1985)].
[10]H. Takahashi, Fusion Technol. **9**, 328 (1986).
[11]R. Abrines and I. C. Percival, Proc. Phys. Soc. London **88**, 861 (1966).
[12]J. S. Cohen and G. Fiorentini, Phys. Rev. A **33**, 1590 (1986).
[13]L. M. Raff, D. L. Thompson, L. B. Sims, and R. N. Porter, J. Chem. Phys. **56**, 5998 (1972).
[14]R. Abrines and I. C. Percival, Proc. Phys. Soc. London **88**, 873 (1966).
[15]M. Leon and H. A. Bethe, Phys. Rev. **127**, 636 (1962).
[16]R. L. Becker and A. D. MacKellar, J. Phys. B **17**, 3923 (1984).
[17]I. C. Percival and D. Richards, Adv. At. Mol. Phys. **11**, 1 (1975).
[18]Based on the size of the stripping cross section and simple geometric considerations, multiple scattering with both nuclei in the molecular target is not expected to be significant. Furthermore, the target rovibrational structure is not expected to be important since the collision energy greatly exceeds the molecular binding energy.