Charge transfer and ionization in collisions of $\alpha\mu$ with all elements

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Cross sections are determined for stripping (charge transfer and ionization) of the $\alpha\mu$ ion in collisions with a number of elements. The calculations are done with the classical-trajectory Monte Carlo method using the Thomas-Fermi model for the neutral-atom target. The total stripping cross sections are shown to differ only slightly from those for collisions with the bare nuclei. A simple analytic formula is given for evaluation of the stripping cross section for any target element. Finally, the results are applied to stopping and stripping of $\alpha\mu$ ions in several metallic foils.

I. INTRODUCTION

Over a hundred d-t fusions have been experimentally observed to be catalyzed by a single negative muon.[1,2] Under optimal conditions of density, tritium fraction, and temperature, the number of fusions is most strongly limited by the probability ω_s that the muon sticks to the fusion α particle to form muonic helium. The value of ω_s has been indirectly obtained by analysis of the time intervals between successive neutrons.[1,2] There is now interest in a direct determination of ω_s by detection of the charged particle products of the fusion reaction;[3,4] barring corrections, then $\omega_s = n_{\alpha\mu}/(n_\alpha + n_{\alpha\mu})$. However, corrections are generally required because of the different stopping rates of the singly and doubly charged ions as well as the possibility that the muon may be stripped from $\alpha\mu$. For example, in one proposed experiment, the charged particles will pass through a thin window and be detected in coincidence with the neutron.[3] To design and correct for the window, its stopping and stripping properties are required. The stopping power is already well known since the small $(\alpha\mu)^+$ ion behaves like a proton in this respect. The stripping has been previously calculated for only the hydrogenic isotopes present in a pure muon-catalyzed fusion target,[5,6] and not for the higher-Z elements of suitable materials.

In the present work, the cross sections for stripping of $\alpha\mu$ by several elements with $1 < Z \leq 92$ are calculated. At high velocities (in particular, at the recoil velocity of $5.83\alpha c$ in d-t fusion), ionization of the muon is the most probable stripping mechanism. At lower velocities, depending on Z, charge transfer dominates. The cross sections are found to vary smoothly with Z, so it is not actually necessary to carry out the scattering calculation at every Z. The Thomas-Fermi model is used for the target atom, and the ionization and charge-transfer cross sections are calculated by the classical-trajectory Monte Carlo (CTMC) method. For comparison, the analogous cross sections for two bare nuclear targets are also calculated. The CTMC method has been used previously for $\alpha\mu$ collisions with hydrogenic targets and found to give good results except at low velocities, $v \lesssim 1\alpha c$.[6] The inaccuracy at low velocities is due in part to transfer into classical orbitals of hydrogen more bound than the true ground state. This situation does not occur in transfer to higher-Z elements, and the cross sections are expected to be more reliable for the full range of velocities.

II. THEORY

A. Potential energy

The actual atomic targets are approximated by the Thomas-Fermi atomic model. Of course, the Thomas-Fermi approximation is not accurate for low-Z atoms and does not reflect the shell structure of actual atoms. However, these limitations are not expected to affect the present calculations adversely. Previous calculations have shown that electron shielding has a negligible effect on the stripping of $\alpha\mu$ by hydrogen,[7] and the same conclusion can be expected to apply to other low-Z atoms. For high-Z atoms, the electron shielding is important, but the electron binding energies *per se* are not; hence the lack of shell structure and the overestimate of electron density very near the nucleus in the Thomas-Fermi atom are not expected to be serious defects.

For use in CTMC calculations, which require large numbers of evaluations of the derivative of the potential, it is convenient to have a simple analytic approximation to the potential. Such a form was derived by Sommerfeld[8] and is used in the present work. The Thomas-Fermi potential (for a *positive* singly charged particle at distance r from the charge-Z nucleus of the neutral atom) is approximated by

$$V = \frac{Z}{r}\phi(1+\phi^{\lambda_+/3})^{\lambda_-/2} \tag{1}$$

with derivative

$$\frac{dV}{dr} = -\frac{V}{r}\left[1+\frac{3}{1+\phi^{\lambda_+/3}}\right], \tag{2}$$

where

$$\phi = \frac{81\pi^2}{8}\frac{1}{Zr^3} \tag{3}$$

and

$$\lambda_\pm = \tfrac{1}{2}(-7 \pm \sqrt{73}) . \tag{4}$$

This approximation has the correct (Thomas-Fermi) behavior in the limits $r \to 0$ and $r \to \infty$ and is within approximately 10% of the exact Thomas-Fermi result over the entire range.[9]

B. CTMC method

The CTMC method has been described in detail many times so will only be sketched here.[10] The initial conditions of the $\alpha\mu$ system are selected at random from a microcanonical distribution having the energy of the ground-state muonic helium ion. The impact parameter (squared) of the collision is selected at random from a range of distances, and this range is increased until convergence is attained. Enough trajectories are run in each range to keep the relative error [1 unit of standard deviation (s.d.)] of the total stripping cross section at 5% in most cases. The total potential energy is the superposition of the Coulomb potential between the α and μ^- with the Thomas-Fermi potentials of the α and μ^- in the field of the atomic target. Hamilton's classical equations of motion for the three-body system are numerically integrated until the outcome of the trajectory is clear. The final-state determination is analogous to that depicted in Fig. 1 of Ref. 10 with the factor γ there, used to compare internal energies with the external potentials, set to 0.2. In the calculations done with a bare-ion target, considerably longer integrations are required and γ was increased to 0.3.

III. RESULTS AND DISCUSSION

The total stripping (muon transfer plus ionization) cross sections calculated for $\alpha\mu$ colliding with several neutral atoms are shown in Fig. 1 over the range of velocities of concern in muon-catalyzed fusion. The cross section tends to peak at velocities of ~ 2 a.u. and is rather flat for the higher-Z elements.[11] For comparison, the stripping cross section for $\alpha\mu + \mathrm{H}$ obtained by conversion of $\mathrm{He}^+ + \mathrm{H}^+$ experimental data,[6] which is presumably more accurate than the CTMC method, is shown by the dashed curve. It is in quite satisfactory agreement with the CTMC calculation except at velocities ~ 1 a.u. The main reason for the discrepancy at low velocities is that muon transfer, which tends to go into orbitals between those that would preserve the energy and size of the original orbital, leads classically to orbitals more tightly bound than the true ground state of the lower-Z target. This illicit transfer causes the cross section to be overestimated. Such a situation does not arise in collisions with atoms of equal or higher Z. Empirically we obtain $\bar{n} \simeq Z^{0.75}$ at the higher velocities and $\bar{n} \simeq Z^{0.75}/\sqrt{2}$ at $v = 1$. Hence the stripping cross sections at $v \sim 1$ are expected to be more reliable for elements with $Z > 1$ than for hydrogen but should still be used with some caution since molecular effects become important at velocities below the muon orbital velocity (2 a.u.).

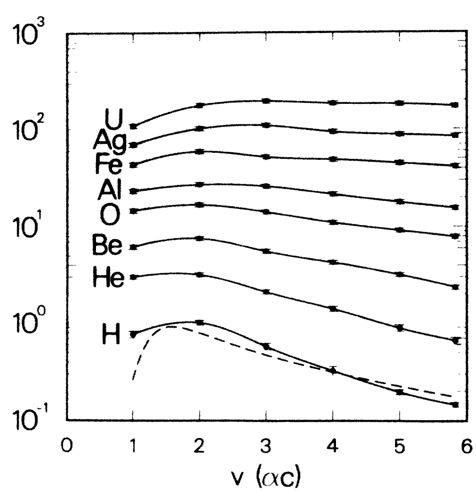

FIG. 1. Cross sections for stripping of $\alpha\mu$ by $_1\mathrm{H}$, $_2\mathrm{He}$, $_4\mathrm{Be}$, $_8\mathrm{O}$, $_{11}\mathrm{Al}$, $_{26}\mathrm{Fe}$, $_{47}\mathrm{Ag}$, and $_{92}\mathrm{U}$ as a function of velocity (units of μa.u.). The data points with statistical (1 s.d.) error bars are from CTMC calculations. The dashed curve is the $\alpha\mu + \mathrm{H}$ cross section obtained by conversion of $\mathrm{He}^+ + \mathrm{H}^+$ data.

Though the energy dependences of the stripping cross sections are fairly flat, the same is not true of the separate transfer and ionization cross sections. The ratios $\sigma_{\mathrm{ion}}/\sigma_{\mathrm{st}}$ are shown as a function of velocity in Fig. 2. The passage from transfer to ionization occurs over a fairly narrow velocity range. The CTMC method is particularly advantageous here in that it treats the charge transfer and ionization processes simultaneously. While for hydrogen charge transfer is rather unimportant as a stripping mechanism, it is important even at $v \sim 6$ a.u. for the high-Z elements. Of course, an ionized muon will usually be subsequently captured by the host element; however, the orbital into which a free muon is captured can be quite different from the orbital to which transfer occurs. Direct capture tends to preserve the energy and size of the *displaced electron*. For example, capture of a free muon by hydrogen[10] occurs with $\bar{n} \simeq 14$ rather than the $\bar{n} \simeq 1$ of transfer from $\alpha\mu$.

The calculations discussed thus far were done using the Thomas-Fermi model for the target atoms. Though the actual collisions do occur with neutral targets and the

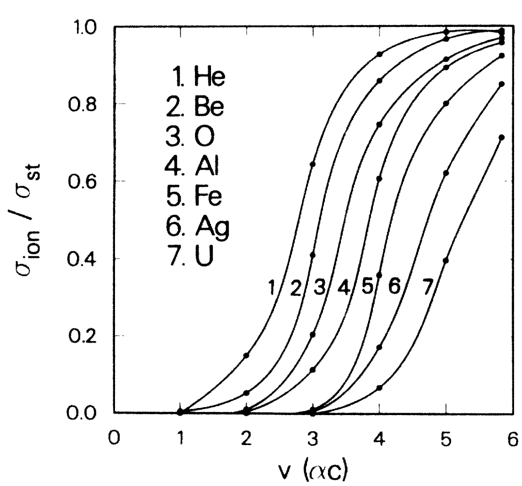

FIG. 2. Fraction of stripping cross section that is ionization, as a function of velocity.

scattering calculation is simpler in the absence of the long-range Coulomb interaction, it is of interest to inquire into the effect of the electron shielding. For this purpose, the CTMC method was also applied to the collisions of $\alpha\mu$ with bare Al and U ions. For Al, the charge transfer and ionization cross sections obtained with the bare target agree with those for the neutral target within statistical errors ($\sim 5\%$). The results for uranium, which should be most extreme, are shown in Fig. 3; here the total stripping results differ slightly but significantly. The stripping by the bare ion is greater except at the lowest velocity. At the higher velocities, little deflection of the $(\alpha\mu)^+$ ion occurs and the stronger potential of the bare U^{92+} enhances stripping. However, at $v=1$ the effect of deflection of the $(\alpha\mu)^+$ by the long-range repulsive Coulomb potential becomes more important and starts to prevent the ion from penetrating to distances where the field is strong enough for stripping. The separate transfer and ionization components depend much more on the electron shielding than does their sum. The stronger attraction of the bare nucleus is able to bind some muons that escape the shielded nucleus. The type ionization that is occurring in the latter case is sometimes termed "charge transfer to the continuum." It is amusing to notice that the similarity of the cross sections for neutral atoms and bare nuclei offers an experimental possibility not easily achieved with normal atoms, namely the measurement of a cross section for an effectively bare high-Z nucleus.

The regular dependence of the stripping cross sections on Z is already suggested by the curves in Fig. 1. This dependence can be generalized in a form convenient for interpolation. In Fig. 4, σ_{st}/Z for all the elements in Fig. 1 is plotted versus v^2/Z. In order to fill in this plot, calculations were also done at $v=10$ and 0.6 a.u. For $v^2/Z \gtrsim 4$ the stripping cross section is proportional to Z^2/v^2. This usual classical relation is expected to be sufficiently accurate for velocities up to ~ 6 a.u. though the quantum-mechanical dependence in the true high-

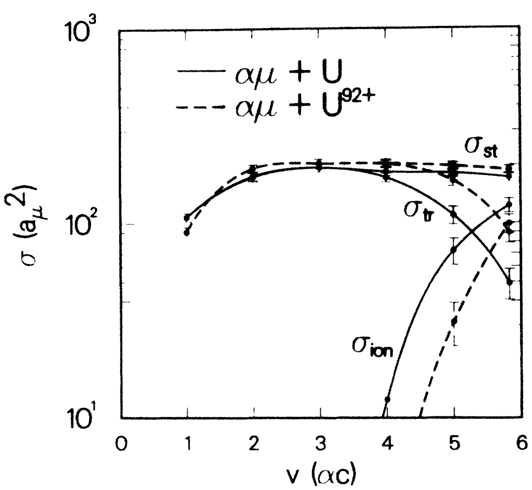

FIG. 3. Cross sections for stripping, charge transfer, and ionization of $\alpha\mu$ by the neutral uranium atom (solid curves) and the completely stripped uranium ion (dashed curves).

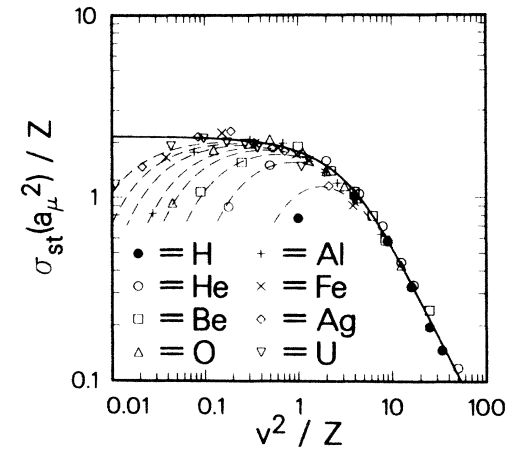

FIG. 4. Reduced $\alpha\mu$ stripping cross section (σ_{st}/Z) as a function of v^2/Z (units of μa.u.). The solid curve is Eq. (5) with reduced mass $M \rightarrow \infty$. The dashed curves are Eq. (5) with M calculated from the atomic weights of $_1H$, $_2He$, $_4Be$, $_8O$, $_{11}Al$, $_{26}Fe$, $_{47}Ag$, and $_{92}U$, from right to left.

velocity limit has a $\log v$ factor. At lower velocities, experience with stripping of the normal H atom[12] would suggest that the cross section becomes linear in Z and *independent* of v, i.e., constant in terms of the reduced variables in Fig. 4. The beginning of such behavior is clearly seen in Fig. 4; however, as v is decreased further the cross section starts to fall in a Z-dependent fashion. This falloff turns out to be due to deflection by the repulsive Coulomb potential and hence depends on the reduced mass as well as Z. At first glance this might be considered surprising, since it is well known that straight-line trajectories are a good approximation at even lower velocities in normal ion scattering and, furthermore, that the cross sections for normal and muonic atoms are frequently related by simply scaling to the appropriate atomic unit. The explanation is that such a relation really requires scaling of the interatomic reduced mass, as well as the intraatomic reduced masses. However, in the actual collisions the distance of approach is smaller (by m_e/m_μ) but the nuclear masses are unchanged; hence deflection is much more important for muonic atoms than for normal atoms.

Nevertheless, the plot in terms of the reduced variables, σ_{st}/Z versus v^2/Z, is useful. We generalize the usual analytic form, which behaves as $(v^2/Z)^{-1}$ at high v^2/Z and approaches a constant at lower v^2/Z, by adding a third factor to cut off the cross section at low v^2/Z. The analysis in the Appendix suggests a factor $\exp[-a/(MZ^{0.5}X)]$, where M is the interatomic reduced mass, X is the reduced variable v^2/Z, and a is a constant. In practice, we find that a slightly different exponent of Z gives a better universal fit. The fit obtained, shown in Fig. 4, is

$$\frac{\sigma_{st}}{Z} = \frac{c}{X}\exp\left[-\frac{a}{MZ^{0.6}X}\right](1-e^{-bX}) , \qquad (5)$$

with $c=5.4$, $b=0.4$, and $a=0.44$ for M in amu. Note that this form becomes c/X at large X, bc at intermediate

X, and $bc \exp[-a/(MZ^{0.6}X)]$ at small X.

This fit can be seen in Fig. 4 to be quite adequate except for $\alpha\mu + \mathrm{H}$ at $v \sim 1$ a.u. (The statistical uncertainties in σ_{st} are 5% except for $v = 0.6$ where they are 10%.) The unreliability of the classical method for $\alpha\mu + \mathrm{H}$ at $v < 2$ a.u. has already been commented on. The inadequacy of Eq. (5) for even the CTMC results on $\alpha\mu + \mathrm{H}$ at $v = 1$ is for a similar reason—transfer to the lower-Z hydrogen atom, unlike all the other atoms, is energetically uphill. Classically there is no rigid threshold, but the cross section still cuts off at low energies though not as abruptly as the true quantum-mechanical behavior.

In light of the small difference between the bare-ion and shielded-ion results, Eq. (5) can be further generalized to include excited states of the $\alpha\mu$ projectile. The exact scaling relation for the pure Coulomb problem (which we do not rigorously have here since the electrons are not simultaneously excited) states that $n^{-4}\sigma_{\mathrm{st}}^{(n)}(v/n)$ is constant[13] (for given Z). Hence for $\alpha\mu$ excited to principal quantum level n with a statistical mixture of l, we can obtain $\sigma_{\mathrm{st}}^{(n)}/(n^4 Z)$ simply by reinterpreting X in Eq. (5) as $X \equiv n^2 v^2/Z$. The CTMC method is not as good for l-specific cross sections, but this is not a drawback as long as the l-mixing cross sections are large.

IV. APPLICATION

The above results can be applied to stripping by impurities or in uniform materials. Compounds can be accurately described as linear combinations of the constituent atoms since only the shielding close to the nuclei is effective. If the $\alpha\mu$ ion is to be stripped, the action must occur before the ion is slowed to $v \lesssim 1$ a.u. since the Coulomb repulsion causes the cross sections to decrease rapidly at lower velocities and also the range at low velocities is short. Hence the fate of $\alpha\mu$ depends on the competition between the stripping and stopping cross sections. The energy loss (per unit distance x) is described by

$$\frac{dE}{dx} = -NS \;, \tag{6}$$

where S is the stopping power of the medium at number density N. Designating the unstripped fraction of $\alpha\mu$ by F, we have

$$\frac{dF}{dx} = -N\sigma_{\mathrm{st}}F \;. \tag{7}$$

Note that S and σ_{st} depend on E; the stopping powers are taken from the tabulation by Andersen and Ziegler.[14] The results for stripping in several elemental materials are shown in Fig. 5. The densities are taken to be the usual densities of the metals and the liquid densities of the normal gases. The initial energy of $\alpha\mu$ is 3.47 MeV; the circles on the curves designate where this energy has been degraded to 3.0, 2.5, 2.0, 1.5, 1.0, and 0.5 MeV.

For hydrogen, helium, and beryllium, Fig. 5 shows that significant fractions of the $\alpha\mu$ ions are stopped unstripped. For silver and gold, the $\alpha\mu$ ions are completely stripped while they still have well over 1 MeV of kinetic energy left. Aluminum and iron lie in between, the stopping and stripping distances being about equal. Unfortunately for muon catalyzed fusion, which is done with as pure a deuterium-tritium mixture as possible, stripping is least in hydrogen. (Deuterium and tritium differ only slightly from protium in this respect.) However, the heavy metals do offer interesting possibilities for stripping the $\alpha\mu$ ion and subsequent observation of the free α particle or of muonic x rays from the captured muon.

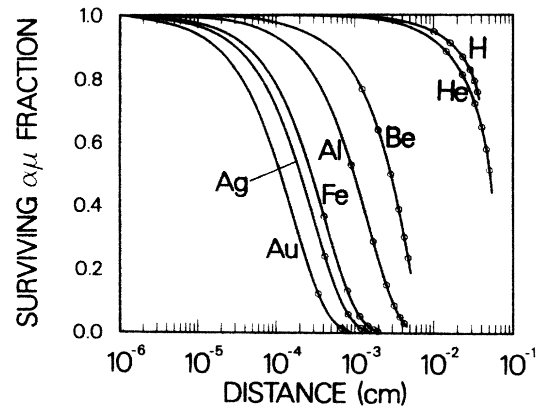

FIG. 5. Surviving (unstripped) $\alpha\mu$ fraction as a function of depth in gold, silver, iron, aluminum, and beryllium foils, and in liquid helium and hydrogen. The initial $\alpha\mu$ ion energy is 3.47 MeV; the circles on each curve show where the ion energy has been degraded to 3.0, 2.5, 2.0, 1.5, 1.0, and 0.5 MeV.

ACKNOWLEDGMENT

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APPENDIX: BEHAVIOR OF THE CROSS SECTION AT LOW ENERGY

This appendix derives the analytic dependence of Eq. (5) used to give a general fit of all the muon stripping cross sections (except that of $\alpha\mu + \mathrm{H}$ at $v \lesssim 1$). A bare target is sufficient for this purpose. At high energies, it is well known that $\sigma_{\mathrm{st}} \sim Z^2/v^2$ classically, so no further discussion is needed for this regime. At low energies, we consider the muon "reaction coordinate" as the ion Z approaches the $\alpha\mu$ at a velocity slower than that of the muon in the ground state of $\alpha\mu$. We start by assuming a straight-line trajectory and will later consider the modification imposed by deflection in the repulsive Coulomb field. Following Haff *et al.*,[15] we take a model in which the muon is transferred to the higher-Z nucleus when its energy just exceeds the barrier between the nuclei as shown schematically in Fig. 6(a). By symmetry, the saddle point through which the muon is transferred must lie on the α-Z axis; the potential of the muon along this axis is given by

$$V(R,r) = -\frac{2}{r} - \frac{Z}{|R-r|} \;, \tag{A1}$$

where r and R are the positions of the muon and Z, respectively, relative to the α. The largest R at which this

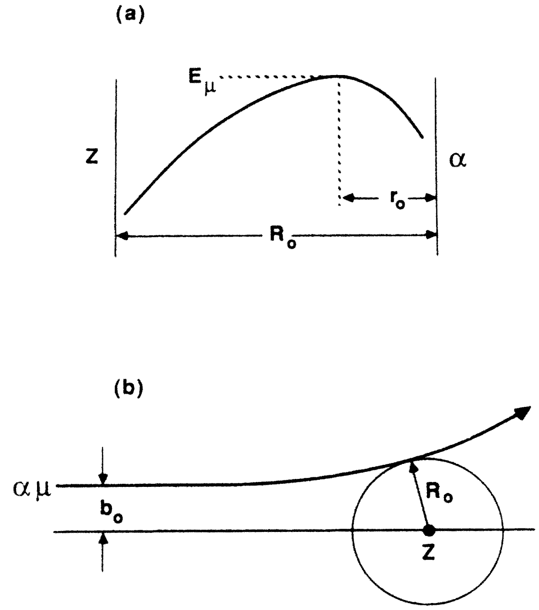

FIG. 6. Schematic diagrams of (a) barrier for transfer between nuclei and (b) trajectory deflection.

transfer can occur is obtained by setting

$$\frac{\partial V}{\partial r}=0 \tag{A2}$$

for fixed R, to obtain r_0 as a function of R, and then solving

$$V(R,r_0)=E_\mu \tag{A3}$$

for R_0. Equation (A2) gives

$$r_0=\frac{R}{1+(Z/2)^{1/2}} \ . \tag{A4}$$

The muon remains much closer to the α particle until the barrier is suppressed and transfer occurs (i.e., the transfer cross section is much larger than the size of the $\alpha\mu$ ion), so we have

$$E_\mu \simeq -E_b - \frac{Z}{R} \ , \tag{A5}$$

where E_b is the binding energy of the $\alpha\mu$ ground state. In the classical microcanonical distribution, an average of half the muon orbital kinetic energy is in angular motion, which does not contribute to the transfer, so it is appropriate to increase E_b in (A5) from 2 to 3 μa.u. Equation (A3) then yields

$$R_0=\tfrac{2}{3}[1+(2Z)^{1/2}] \ . \tag{A6}$$

In this crude model, muon transfer occurs if $R \le R_0$ is reached. Remember that this description is only valid for $v \lesssim 2$ a.u. and $Z>2$. Because of the latter condition we take simply

$$R_0 \simeq \frac{2\sqrt{2}}{3} Z^{1/2} \ . \tag{A6$'$}$$

Now we turn to the reduced-mass dependence. Muon transfer is assumed to occur in all collisions at impact parameters $b<b_0$, where b_0 is the maximum impact parameter that will allow the distance R_0 to be reached as shown schematically in Fig. 6(b). Hence

$$\tfrac{1}{2}Mv^2=\frac{Z}{R_0}+\frac{Mb_0^2v^2}{2R_0^2} \ . \tag{A7}$$

Solving (A7) for b_0 and using (A6$'$) for R_0, we obtain an approximation to the cross section at low energy,

$$\sigma_{\rm low}=\pi b_0^2=\frac{8\pi}{9}Z\left[1-\frac{3}{\sqrt{2}}\frac{Z^{1/2}}{Mv^2}\right] \ . \tag{A8}$$

For $Mv^2 \gg Z^{1/2}$, this gives $\sigma_{\rm low}/Z \simeq 2.8$, in rather good agreement with the peak in Fig. 4. Of course, the actual cross section does not go identically to zero as this expression does. We remedy this defect by noting that (A8) is the first term in the expansion of an exponential, so

$$\sigma_{\rm low} \simeq \frac{8\pi}{9}Z \exp\left[-\frac{3}{\sqrt{2}}\frac{Z^{1/2}}{Mv^2}\right] \ . \tag{A9}$$

Finally, we generalize this expression to include the high-energy behavior as well by writing

$$\frac{\sigma_{\rm st}}{Z} \simeq \frac{c}{X}\exp\left[-\frac{a}{MZ^{0.5}X}\right](1-e^{-bX}) \ , \tag{A10}$$

where $X \equiv v^2/Z$ and we have replaced the constants by adjustable parameters. In the numerical fit, it was found that $Z^{0.6}$, instead of $Z^{0.5}$, in the middle factor provides a somewhat better representation (this minor difference appears to be due to the electron shielding that has been ignored in this simple derivation).

It should be emphasized that the purpose of this appendix is merely to motivate the analytic form used to fit the stripping cross sections and perhaps to contribute some physical insight. The crude approximations made here in no way affect the CTMC calculation of these cross sections.

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[11]Muonic atomic units ($\hbar = e = m_\mu = 1$) are used except where otherwise stated: distance $1a_\mu = 2.56\times 10^{-11}$ cm, velocity 1 μa.u. = 1 a.u. $= \alpha c = 2.19\times 10^{8}$ cm/s, cross section $1a_\mu^2 = 6.55\times 10^{-22}$ cm^2, energy 1 μa.u. = 5627 eV.

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