Variational sticking-fraction calculations for the ground state of the $td\mu$ molecular ion

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We have used variational wave functions for the ground state of the $td\mu$ molecular ion to find the probability that after the *t-d* fusion the system will be in a state with the muon bound to the α particle. This probability, known as the sticking fraction, was found to be 0.8860×10^{-2}.

I. INTRODUCTION

Recently there has been a great deal of interest in muon-catalyzed fusion (μCF) of the hydrogen isotopic nuclei. The most promising of these fusion reactions is

$$td\mu \xrightarrow{\omega_s^0} \alpha\mu + n + 17.6\ \text{MeV}\ , \quad (1a)$$

$$td\mu \xrightarrow{1-\omega_s^0} \alpha + \mu + n + 17.6\ \text{MeV}\ . \quad (1b)$$

Were it not for reaction (1a), each muon could induce roughly 1000 fusions in its lifetime. However, experiments and calculations have indicated that for about 1% of the reactions the muon sticks to the α particle. The probability that this will occur is the initial sticking fraction ω_s^0 and it can be calculated using the wave function of the $td\mu$ ion. If this function is taken in the Born-Oppenheimer approximation,[1,2] a sticking fraction of 1.2×10^{-2} is obtained. Later calculations including nonadiabatic effects gave values of the sticking fraction of $0.895\times10^{-2}\pm0.004\times10^{-2}$ (Ref. 3), $(0.845\times10^{-2}$ (Ref. 4), and 0.897×10^{-2} (Ref. 5). Each of the above results was obtained with entirely different techniques, so the agreement may be considered to be quite good. On the other hand, the results of Ref. 4 are an order of magnitude outside the error bars given in Ref. 3. The authors of Ref. 4 estimate the accuracy of their value to be much better than 3%, which adds error bars much smaller than $\pm0.03\times10^{-2}$ to their value. In Ref. 5 an accuracy of about $\pm0.01\times10^{-2}$ is suggested. The above differences between the literature values of ω_s^0 are large enough to warrant an accurate calculation of this quantity with a systematic convergence analysis. Since at present sticking seems to determine the efficiency of μCF, the number of fusions a single muon can induce is approximately inversely proportional to the effective sticking fraction. The effective sticking fraction includes the reactivation of muons from the $\alpha\mu$ particles in the process of collisions in the mixture; $\omega_s=(1-R)\omega_s^0$, where R is the so-called reactivation coefficient. The latest theoretical value of this coefficient is $R=0.36$ (Ref. 6) at a density of $\phi=1.2$ liquid-hydrogen densities. Therefore the above cited calculations of ω_s^0 lead to $\omega_s\sim0.54$ to 0.57×10^{-2}. This is substantially more than the recent experimental results, $(0.35\pm0.07)\times10^{-2}$ [Ref. 7(a)] and $(0.45\pm0.05)\times10^{-2}$ [Ref. 7(b)].

In this work we describe sticking-fraction calculations for the $td\mu$ ground state. Although reasons for the large discrepancy between experiment and theory may be outside a Coulombic description of the system, a definitive sticking-fraction value at this level is important before investigating the influence of other forces. We will use variational, generalized Hylleraas-type functions to describe the ground state of $td\mu$. Very large basis sets have been employed to obtain good convergence. The energy of the $td\mu$ ground state given by these functions[8] is orders of magnitude more accurate than literature data. The effects of imposing two-body cusp conditions have been carefully examined.

II. THEORY

We will consider the partial sticking fractions which are equal to the transition probabilities between the ground state of the $td\mu$ molecular ion and the bound states of the $\alpha\mu$ hydrogenlike ion. The high rate of fusion compared to molecular processes allows us to use the sudden approximation. The correction to the sudden approximation has been estimated to be less than 3% of ω_s^0 (Ref. 4). Also, effects due to the finite size of the compound nucleus ^{5}He have been ignored, since the characteristic nuclear scale is roughly $0.02a_\mu$, where a_μ is the Bohr radius of the muon.[2]

The final wave function may be written as

$$\Psi_f(\mathbf{r}_\mu,\mathbf{r}_\alpha,\mathbf{r}_n)=e^{i\mathbf{p}_n\cdot\mathbf{r}_n}e^{i\mathbf{p}_{\alpha\mu}\cdot\mathbf{r}^c_{\alpha\mu}}\Psi_\beta(\mathbf{r}_{\alpha\mu})\ , \quad (2)$$

where $\mathbf{p}_n$ and $\mathbf{p}_{\alpha\mu}$ are the momenta of the neutron and of the $\alpha\mu$ ion, respectively; $\mathbf{r}_\mu$, $\mathbf{r}_\alpha$, $\mathbf{r}_n$, and $\mathbf{r}^c_{\alpha\mu}$ are positions of the muon, α particle, neutron, and center of mass of $\alpha\mu$, respectively, in a laboratory-fixed coordinate system; and $\mathbf{r}_{\alpha\mu}=\mathbf{r}_\alpha-\mathbf{r}_\mu$. Here and elsewhere in this paper, unless otherwise indicated, we have used units such that $\hbar=e=m_{t\mu}=1$, where $m_{t\mu}$ is the $t\mu$ reduced mass. For bound states of $\alpha\mu$, Ψ_β are hydrogenic-type functions.

$$\Psi_\beta(\mathbf{r})=\Psi_{nlm}(\mathbf{r})=R_{nl}(r)Y_{lm}(\theta,\phi)\ , \quad (3)$$

where R_{nl} are the radial wave functions and Y_{lm} are spherical harmonics. For the continuous spectrum of $\alpha\mu$, R_{nl} must be replaced by Coulomb wave functions. If we assume that the center of mass of the whole system is at

rest, the initial state can be described by a function $\Psi_i(\mathbf{r}_{t\mu},\mathbf{r}_{td})$, where $\mathbf{r}_{xy}$ denotes the vector connecting particles x and y. In the sudden approximation the amplitude of transition to a final state is proportional to the overlap between the initial and final wave functions taken at the point of coalescence of d, t, α, and n,

$$F_\beta = N\int \Psi_\beta^*(\mathbf{r}_{\alpha\mu}) e^{-i\mathbf{p}_n\cdot\mathbf{r}_n} e^{-i\mathbf{p}_{\alpha\mu}\cdot\mathbf{r}^c_{\alpha\mu}} \times \Psi_i(\mathbf{r}_{t\mu},\mathbf{r}_{td})\,|_{\mathbf{r}_\alpha=\mathbf{r}_n=\mathbf{r}_t=\mathbf{r}_d} d\mathbf{r}_\mu d\mathbf{r}_\alpha \,, \tag{4}$$

where N is a normalization factor. Since conservation of momentum requires that $\mathbf{p}_n=-\mathbf{p}_{\alpha\mu}$, integration over $\mathbf{r}$ gives

$$F_\beta = N\int \Psi_\beta^*(\mathbf{r}) e^{-i\mathbf{q}\cdot\mathbf{r}} \Psi_i(\mathbf{r},0) d\mathbf{r} \,, \tag{5}$$

where $\mathbf{r}\equiv\mathbf{r}_{\alpha\mu}$ and

$$\mathbf{q} = \frac{m_\mu}{m_\mu+m_\alpha}\mathbf{p}_n \,. \tag{6}$$

A relativistic calculation of $q=|\mathbf{q}|$ presented in the Appendix results in $q=6.0626$. The partial sticking fraction for a state nl is now defined as a branching ratio

$$\omega_{nl} = \sum_m \frac{|F_{nlm}|^2}{\sum_\beta |F_\beta|^2} \,. \tag{7}$$

The total initial sticking fraction is

$$\omega_s^0 = \sum_{n,l} \omega_{nl} \,. \tag{8}$$

Neglecting the dependence of q on the energy of the final state and using the closure relation for the set $\{\Psi_\beta\}$, we get

$$\omega_{nl} = \sum_m \frac{|F_{nlm}|^2}{\langle\Psi_i(\mathbf{r},0)|\Psi_i(\mathbf{r},0)\rangle} \,. \tag{9}$$

Introducing

$$\psi_i(\mathbf{r}) = \frac{\Psi_i(\mathbf{r},0)}{[\langle\Psi_i(\mathbf{r},0)|\Psi_i(\mathbf{r},0)\rangle]^{1/2}} \,, \tag{10}$$

we may write Eq. (9) in the familiar form

$$\omega_{nl} = \sum_m \left|\int d^3r\, R_{nl}^*(r) Y_{lm}^*(\theta,\phi) e^{-i\mathbf{q}\cdot\mathbf{r}} \psi_i(r)\right|^2 . \tag{11}$$

Introducing the partial-wave expansion for $e^{i\mathbf{q}\cdot\mathbf{r}}$ and integrating over the angles gives

$$\omega_{nl} = (2l+1)\left|4\pi\int dr\, r^2 R_{nl}(r) j_l(qr)\psi_i(r)\right|^2 , \tag{12}$$

where $j_l(qr)$ is the spherical Bessel function.

The sticking fraction is strongly dependent on the value of the initial wave function at the point of dt coalescence. A correct behavior of the wave function in this region can be secured by imposing proper cusp conditions. The two-body cusp conditions are

$$\lim_{r_{xy}\to 0} \frac{\delta}{\delta r_{xy}} \ln\Psi_i = Z_x Z_y \frac{m_{xy}}{m_{t\mu}} \,, \tag{13}$$

where m_{xy} is the reduced mass of particles x and y, and Z_x is the charge of particle x. The wave function satisfying these conditions is

$$\Psi_i = \sum_{j=l}^{N} c_j (d_j + d_j' r_{t\mu})(e_j + e_j' r_{d\mu})(f_j + f_j' r_{td}) \times r_{t\mu}^{l_j} r_{d\mu}^{m_j} r_{td}^{n_j} \exp(-\alpha r_{t\mu} - \beta r_{d\mu} - \gamma r_{td}) \,, \tag{14}$$

where

$$d_j = \begin{cases} 1 \\ 0, \end{cases} \quad d_j' = \begin{cases} \alpha-1 & =0 \\ 1, & l_j>0 \,, \end{cases} \tag{15}$$

$$e_j = \begin{cases} 1 \\ 0, \end{cases} \quad e_j' = \begin{cases} \beta & =0 \\ 1-\dfrac{m_{d\mu}}{m_{t\mu}}, & m_j>0 \,, \end{cases} \tag{16}$$

$$f_j = \begin{cases} 1 \\ 0, \end{cases} \quad f_j' = \begin{cases} \gamma & =0 \\ 1+\dfrac{m_{td}}{m_{t\mu}}, & n_j>0 \,. \end{cases} \tag{17}$$

Our calculations were performed without using cusp conditions, with one condition, $r_{td}\to 0$, and with all three cusp conditions. The coefficients c_j were obtained by a diagonalization of the proper Hamiltonian matrix. Optimal values of the nonlinear parameters were found to be $\alpha=0.749$, $\beta=0.694$, and $\gamma=1.383$ (Ref. 8). Small changes in these parameters had a negligible effect on the energy of the sticking fraction provided that N was large.

Inserting our wave function in the form of Eq. (14) into Eq. (12) leads to integrals of the following type:

$$\int dr\, r^2 R_{nl}(r) j_l(qr) r^m e^{-\alpha r} = (2q)^l N_{nl} \sum_{k=1}^{n-1} A_k \lambda_n^k (-2)^M \times \sum_{L=0,1/2}^{M/2} D_{ML} \frac{a^{2L}(1+M/2+L)!}{(a^2+q^2)^{1+M/2+L+1}} \,, \tag{18}$$

$$a = \alpha + \tfrac{1}{2}\lambda_n \,,$$

$$\lambda_n = \frac{2Z}{n a_{\alpha\mu}}$$

$$N_{nl} = \frac{[Z(n-l-1)!]^{1/2}}{\{n^2 a_{\alpha\mu}[(n+l)!]^3\}^{1/2}} \lambda_n \,,$$

$$A_k = (-1)^{(k-l)} \frac{[(n+l)!]^2}{(k-l)!(n-k-1)!(l+k+1)!} \,,$$

$$M = k-l+m+1 \,,$$

where D_{ML} can be computed recursively,

$$D_{00}=1, \quad D_{1,1/2}=-1, \quad D_{ML}=0 \quad (L<0,\ L>M/2) \,,$$

$$D_{ML} = -D_{M-1,L-1/2} + (L+\tfrac{1}{2}) D_{M-1,L+1/2} \,,$$

or directly

$$D_{ML} = (-1)^{M/2+L} 2^{2L-M} \frac{M!}{(M/2-L)!(2L)!} \,.$$

$Z=2$ is the nuclear charge of the α particle and $a_{\alpha\mu}$ is the Bohr radius of the $\alpha\mu$ atom.

TABLE I. Dependence of the sticking fraction for the 00 state on the size of the basis set and on the cusp conditions. The sticking fractions reported here were obtained as sums of the partial sticking fractions up to $n=30$.

N[a]	l_{max}[b]	n_{max}[c]	max[d]	$10^2\omega_s^0$ A[e]	B[f]	C[g]
23	2	2	4	0.355	0.014	0.051
56	5	5	5	0.007	0.627	0.798
84	6	6	6	0.0001	1.30	0.189
120	7	7	7	0.030	1.04	0.159
157	6	8	8	0.192	1.15	0.557
200	6	9	9	0.729	0.8593	0.844
372	6	9	13	0.945	0.8725	0.868
415	8	12	12	0.8959	0.8845	0.8784
600	9	14	14	0.8842	0.8854	0.8819
746	10	15	15	0.8845	0.8851	0.8858
968	10	15	17	0.8852	0.8850	0.8850
1158	11	16	18	0.8854	0.8850	0.8859
1995	11	16	25	0.885 36		

[a]N is the total number of basis functions.
[b]l_{max} is the maximum power of $r_{t\mu}$ and $r_{d\mu}$.
[c]n_{max} is the maximum power of r_{dt}.
[d]max is the maximum sum of the powers of $r_{t\mu}$, $r_{d\mu}$, and r_{dt}.
[e]No cusp conditions are imposed on the wave function.
[f]The cusp condition as $r_{dt}\rightarrow 0$ is imposed.
[g]The three two-body cusp conditions are imposed.

III. RESULTS

In order to achieve accurate values of the sticking fraction ω_s^0 we used basis sets containing up to 1995 functions. For basis sets larger than 400 functions we had to use double precision of a Cray-2 computer (~ 29 decimal digits) or quadrupole precision of an IBM 3090 computer (~ 32 decimal digits). In Table I we compare sticking fractions calculated with and without cusp conditions for various lengths of the basis set. The sticking fractions reported are the sum of partial sticking fractions ω_{nl} from $n=1$ to 30 and $l=0$ to 4. The values of ω_{nl} for $l\geq 5$ were less than 10^{-10}. The partial sticking fractions decreased less rapidly with increasing n. In the Born-Oppenheimer (BO) approximation the sum of the partial sticking fractions from $n=31$ to ∞ is equal to $0.000\,78\times 10^{-2}$. We have found that for n values ranging from 8 to 30 our

$$\omega_n=\sum_{l=0}^{n-1}\omega_{nl}$$

represent 0.757 of the respective values obtained with the BO approximation. Therefore we multiplied the large-n contribution calculated in the BO approximation by this value, obtaining $0.000\,59\times 10^{-2}$ as the final contribution of the terms with $n>30$. This value must be added to the sticking fractions in Table I. Our final result is then $\omega_s^0=0.885\,95\times 10^{-2}$, i.e., it is the sticking fraction obtained using 1995 basis functions plus the remainder estimated using the scaled Born-Oppenheimer approximation.

The convergence patterns suggest that our ω_s^0 is converged to almost three significant digits. In contrast to the opinion held in Ref. 5, an imposition of the cusp conditions improves the convergence only for small basis sets. For basis sets with fewer than 400 functions the results obtained using no cusp conditions vary wildly, whereas the values with the cusp conditions imposed are relatively stable. The latter sticking fractions are, however, very inaccurate. For larger basis sets, all three types of calculations converge with a similar rate. Reliable values of ω_s^0 are obtained with basis sets with 400 or more terms. Our results show that if the basis set is large enough, the cusp conditions are well satisfied in the variational calculation and that fulfilling the cusp condition only is definitely not sufficient to obtain accurate sticking fraction.

In Table II we compare the energies calculated with and without cusp conditions. For our smallest basis set of 23 functions the result with three cusp conditions is the best, while for medium size basis sets (from $N=84$ to $N=415$) the best is the result with one cusp condition. For all the larger N the energies calculated without cusp conditions are the most accurate. The convergence of energies for large N is drastically reduced when the three cusp conditions are imposed: the accuracy with a given basis set can be as much as five orders of magnitude lower than in a calculation without cusp conditions. There are two competing effects which are responsible for this behavior. The first effect is due to the fact that imposing cusp conditions implies an enriching of the initial basis set. Therefore, for small N the higher powers of the interparticle distances appearing in Eq. (14) improve the quality of the basis set and therefore the energy with cusp conditions is better than without them. For large N, however, this improvement is not important anymore and the constraints imposed on the basis set due to the

TABLE II. Convergence of the binding energies for the 00 state of the $td\mu$ molecule.

	Energy (eV)		
N	A^a	B^a	C^a
23	−290.8	−302.0	−304.7
84	−319.0	−319.13	−318.62
120	−319.121	−319.1367	−318.87
157	−319.1377	−319.1383	−319.03
200	−319.139 68	−319.139 707	−319.08
372	−319.139 728	−319.139 729	−319.118
415	−319.139 751 5	−319.139 751 8	−319.1306
600	−319.139 752 09	−319.139 752 07	−319.1356
746	−319.139 752 14	−319.139 752 12	−319.1372
968	−319.139 752 159	−319.139 752 145	−319.1381
1158	−319.139 752 161	−319.139 752 151	−319.1387
1995	−319.139 752 163		

[a]See Table I.

cusp conditions make the energy less accurate. Hu[5] applied two cusp conditions to her wave function: the condition as $r_{dt} \to 0$ and the three-body condition. The energy obtained in Ref. 5 using 500 basis functions, −319.134 19 eV, is between the energies we found using 415 and 600 basis functions and three cusp conditions.

Morgan[9] has pointed out that when the sticking fraction is found using the sudden approximation, it may be thought of as the expectation value of the δ function $\delta(r_{dt})$. The error in this expectation value may then be related to the error in the energy. If the energy has converged to N places, the sticking fraction may be expected to have converged to $N/3$ places. By this argument, our final sticking fraction is accurate to at least three significant figures. Also, by the same argument, for larger N the sticking fractions obtained using no cusp conditions should be far more reliable than those obtained using three cusp conditions. A comparison of the results of Tables I and II shows indeed that the calculation which gives a more accurate energy in most cases also gives a more accurate sticking fraction. On the other hand, for N from 56 to 372 and for $N=746$, the sticking fraction with three cusp conditions is better than the one with no cusp condition—despite much worse energy in the former case. Thus imposing cusp conditions clearly can make the sticking fraction better than the energy criterion would indicate. In very large basis sets, however, the cusp conditions are very accurately reproduced without imposing them explicitly on the basis functions and the energy criterion determines the accuracy of the sticking fractions. Increasing the size of the basis set by a factor of almost 2, i.e., from $N=1158$ to $N=1995$, did not change the first four digits of the sticking fraction which gives us a high degree of confidence in the correctness of our estimation of accuracy presented above.

In Table III we compare our results with literature data. Our final value of ω_s^0 lies between the value of Bogdanova *et al.*[4] and the values of Ceperley and Alder[3] and Hu.[5] We believe that our ω_s^0 is accurate to three digits, which implies that the relative errors of the literature values are about 2% to 4%. The results of Bogdanova *et al.*[4] obtained using a numerical solution in the adiabatic representation are the least accurate.

Each calculation of the sticking fractions includes some estimation of the contribution of large n. In our case the estimated part is only 0.0006×10^{-2} since the calculations have been performed up to $n=30$. As mentioned above, to estimate the remainder we summed the sticking fractions computed in the BO approximation up to infinity. More precisely, we computed exactly these values up to $n=100$ obtaining $\sum \omega_n^{BO}=1.172\,103\times10^{-2}$. From $n=101$ to 10 000 we used the asymptotic formula for ω_n^{BO} given by Bogdanova *et al.*[10] [also Eq. (21) in Ref. 4] which gives a contribution of 0.67×10^{-6}. This formula slightly (and systematically) underestimates the exact values of ω_n^{BO}: for n from 10 to 100, $\omega_n^{BO}/\tilde{\omega}_n^{BO}=1.073$, where the tilde denotes the approximate expression. Thus we multiplied the value obtained above by this ratio which leads to a contribution equal to 0.72×10^{-6}. The contribution of all $n>10\,000$ can be calculated by a further simplification of the Eq. (21) of Ref. 4 to the form $\omega_n^{BO}\sim0.02/n^3$ and employing the Rieman ζ function. Such a procedure shows that this contribution is completely negligible, being equal to 10^{-10}. The final value of the sticking fraction in the BO approximation is $1.172\,18\times10^{-2}$.

Bogdanova *et al.*[4] performed their nonadiabatic calculations up to $n=4$ and estimated the remainder using their formula (21). Unfortunately, the numerical value of 0.0278 for the contribution of the $n>4$ terms in the BO approximation given in Table 2 of Ref. 4 disagrees with our value of 0.0326×10^{-2} calculated with the same equation. (The exact BO contribution for $n>4$ is equal to 0.0350×10^{-2}.) Similarly, we could not reproduce the values given in Table 2 of Ref. 4 for an $n>4$ contribution in the case of the adiabatic calculations. Neither Hu[5] nor Ceperley and Alder[3] explain how they computed the large-n terms.

Our values and literature values for the contribution for $n>4$ are compared in the last row of Table III. In the case of Refs. 3 and 5 the "all other" term contained in fact some contribution from terms with $n\leq4$. To enable a comparison we have subtracted the values of these terms taken from our calculations. The contributions of $n>4$ terms from various papers differ by $\sim0.002\times10^{-2}$. Table III shows that the major source of discrepancies

TABLE III. Comparison of the sticking fractions $10^2\omega_s^0$ obtained in this work using 1995 basis functions and no cusp conditions with literature data.

	Ref. 3	Ref. 4	Ref. 5	Present results
ω_s^0	0.895(4)	0.845	0.897	0.8860
ω_{1s}	0.689	0.6502	0.6932	0.6826
ω_{2s}	0.099	0.0934	0.0992	0.0979
ω_{2p}	0.024	0.0238	0.0241	0.0238
ω_{3s}	0.030	0.0284	0.0302	0.0297
ω_{3p}	0.009	0.0086	0.0087	0.0086
ω_{3d}		0.0003		0.0002
ω_{4s}	0.013	0.0121	0.0128	0.0127
ω_{4p}		0.0037	0.0039	0.0039
ω_{4d+4f}		0.0003		0.0001
ω_{5s}			0.0066	0.0065
$\sum_{n=5}^{30}\omega_n$				0.0259
"All other"[a]	0.031	0.024	0.018	0.0006
$\sum_{n=5}^{\infty}\omega_n$	0.027[b]	0.0241	0.024[c]	0.0265

[a] ω_s^0 minus the sum of all the entries given above.
[b] Obtained by subtracting from the value given in Ref. 3 our contributions of ω_{3d}, ω_{4p}, ω_{4d}, and ω_{4f}.
[c] Obtained by adding to the value given in Ref. 5 the ω_{5s} contribution (from Ref. 5) and subtracting ω_{3d}, ω_{4d}, and ω_{4f}.

between ω_s^0 values is contained in the $1s$ component.

Another question in comparing our data and literature data concerns different nuclear and muon masses used in various works. As shown in Ref. 8, uncertainties in the masses lead to energy changes of the order of 0.1 meV, i.e., they change the eighth digit in the total energy. Thus the different masses may influence only the third significant digit of the sticking fraction. On the other hand, the sticking fraction may be sensitive to the q value used. We found that the plot of ω_s^0 versus q is roughly linear with a slope of about -0.01. The q values used by Ceperley and Alder,[3] Bogdanova *et al.*,[4] and Hu[5] are 6.0639, 6.063, and 6.0638 in our units, respectively. The difference between these values and our value of 6.0626 is due to the different masses and to the inclusion of the ground-state $\alpha\mu$ energy in our calculation of q. Thus the effect on the sticking fraction is of the order of 0.001×10^{-2}. The change in q value would increase the discrepancy between our sticking fractions and those of Refs. 3 and 5.

IV. CONCLUSIONS

We have shown that very accurate values of the initial sticking fraction can be obtained using variational wave functions. The variational method has been considered by many researchers to be an inferior approach for calculating sticking fractions. This was based on an argument that the variational method cannot be sensitive to a region of nuclear coalescence which is unimportant for the state energy. We show that the above opinion is not correct since our values seem to be much more accurate than all the literature data including those obtained with methods supposedly better suited for calculating the sticking fraction.

Our sticking fraction of 0.8860×10^{-2} is accurate to three or four digits and is different from the literature values by 0.011×10^{-2} to 0.041×10^{-2}. Such a difference, of course, does not solve the problem of a large discrepancy between theory and experiment. Our calculations show definitively that the reason for this difference must be sought outside the Coulomb description of the problem. We are presently working on the effects of strong nuclear forces using R-matrix theory.

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APPENDIX

The amount of energy released during fusion is

$$Q=(m_t+m_d-m_\alpha-m_n)^2c=34.402m_e=17.5797\ \text{MeV},$$

where $m_t=5496.899m_e$, $m_d=3670.481m_e$,[11] $m_\alpha=7294.295m_e$,[12] and $m_n=1838.683m_e$.[13] The value of $p=|\mathbf{p}_{\alpha\mu}|=|\mathbf{p}_n|$ which defines q [Eq. (6)] may be found using energy conservation,

$$\frac{Q}{c}=\frac{E_{\alpha\mu}}{c}+[p_{\alpha\mu}^2+(m_\alpha+m_\mu)^2c^2]^{1/2}+(p_n^2+m_n^2c^2)^{1/2}$$
$$-(m_\alpha+m_\mu)c-m_nc\ ,$$

where $m_\mu=206.7686m_e$ and $E_{\alpha\mu}$ denotes the ground-state energy of $\alpha\mu$, $E_{\alpha\mu}=-0.010\,943$ MeV $=0.021\,414m_ec^2$. The value of p can easily be extracted from the above equation giving $q=4.505\,049$ MeV/c. To obtain q in our muonic-atom units, $\hbar=e=m_{t\mu}=1$, we must multiply by

$$1/(101.829\,10\times0.005\,422\,534\,7)^{1/2}=1.345\,745\ ,$$

where the first number in the square brackets is the muon mass in MeV and the second factor is the energy conversion factor. This gives finally $q=6.0626$ (in units of $\mu_\mu=1$, and $q=5.8460$). This value is close to that used by Bogdanova *et al.*[4] Since we include the $\alpha\mu$ binding energy and they do not, it is probable that different nuclear masses were used in Ref. 4. The uncertainties of the nuclear masses change q at the fourth digit.

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