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Variational calculation of the muon–alpha-particle sticking probabilities in the muon-catalyzed fusion $dt\mu \rightarrow \mu\,^4\mathrm{He}+n$

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μ-α sticking probabilities have been calculated for the S state and the P state, using a high-precision three-body variational wave function. The 0.90% S-state sticking probability agrees with previous works using other methods. It is necessary to calculate two sets of sticking probabilities and fusion rates for the $J=1$, $v=0$ state, from which an effective sticking probability of 0.31% is calculated. As in all previous calculations, the traditional sudden approximation is used whenever possible. In addition, it is necessary to average the sticking probability over a small region of nuclear influence instead of evaluating it at the point of nuclear coalescence.

The problem of the muon sticking to the ^{4}He nucleus in the final state of the $dt\mu$ fusion reaction has been an important concern in muon-catalyzed fusion processes. Previous μ-α sticking probabilities were calculated for the S state of the muon molecular systems.[1-4] They range from 1.2%[1,2] to 0.90%.[3,4] They are at least a factor of 2 or more larger than the experimental value.[5]

I report a calculation of the μ-α sticking probabilities and the fusion rates from both the S state and the P state of the $dt\mu$ molecule. The muon molecular wave function is obtained from a three-body variational calculation.[6] However, in Ref. 6, the calculations were carried out without Coulomb cusp constraints. The cusp constraints prove to be essential for the sticking-probability calculations. The details of the cusp constraints and the muon sticking probabilities are given later. The results of the calculations will also be presented. The fusion rates and the S-state muon sticking probability are in good agreement with those of Refs. 3 and 4. Two sets of sticking probabilities and fusion rates for the $J=1$, $v=0$, state have also been obtained. These correspond, respectively, to the initial nuclei being in a relative S or P state. The traditional method cannot be used to calculate the sticking probability for the latter. The traditional method is used whenever possible. In addition, the sticking probabilities and the fusion rates are averaged over a region of the approximate range of the nuclear force instead of evaluating them at the point of nuclear coalescence. From these two sets of sticking probabilities and fusion rates, an overall effective muon-sticking probability of 0.31% is calculated for the $J=1$, $v=0$, state. The best energy for the $J=0$, $v=0$ state is $-319.134\,19$ eV, and for $J=1$, $v=0$ state is $-232.468\,67$ eV.

(a) *S state.* According to the sudden approximation,[7] the sticking amplitude is the overlapping integral

$$A_{if}=\int d^3r\,\phi_i(\mathbf{r})\phi_f(\mathbf{r}) \ . \tag{1}$$

$\phi_f(\mathbf{r})$ is the wave function of a fast-moving $\mu\,^4$He atom with the muon in various hydrogenlike orbits and

$$\phi_i(\mathbf{r})=\lim_{\rho\rightarrow 0}\psi(\mathbf{r},\boldsymbol{\rho})/\left[\int d^3r\,|\psi(\mathbf{r},\boldsymbol{\rho})|^2\right]^{1/2} \ . \tag{2}$$

$\psi(\mathbf{r},\boldsymbol{\rho})$ is the full three-body wave function of the $dt\mu$ molecule.[6] $\mathbf{r},\boldsymbol{\rho}$ are defined as follows:

$$\boldsymbol{\rho}=\mathbf{R}_2-\mathbf{R}_1,\ \mathbf{r}=(\mathbf{R}_3-\mathbf{R}_1+\mathbf{R}_3-\mathbf{R}_2)/2 \ . \tag{3}$$

These are not the Jacobian coordinates for three unequal masses. They are used only to normalize our wave functions so that our fusion rates can be compared directly with those of previous calculations using other methods. m_1, m_2, and m_3 are the masses of the triton, deuteron, and muon, respectively, and $M=m_1+m_2+m_3$. R_1, R_2, and R_3 are the coordinates with respect to a fixed coordinate system. The sticking probability for a transition to a $\mu\,^4$He atom with orbital angular momentum l and total quantum number n is given by[1,3]

$$\omega_{nl}=4\pi(2l+1)\left|\int\phi_i(r)R_{nl}(r)j_l(Qr)r^2dr\right|^2 \ . \tag{4}$$

$R_{nl}(r)$ is the radial function of the $\mu\,^4$He atom, $j_l(Qr)$ is the spherical Bessel function, $Qa_n = 5.844$, and a_n is the muon Born radius. The total sticking probability is $\omega_s = \sum \omega_{nl}$. The three-body wave function for the S state is

$$\psi_S = \sum_{n_1} \sum_{n_2} \sum_{n_3} C_{(n_1 n_2 n_3)} r_{12}^{n_1} r_{13}^{n_2} r_{23}^{n_3} \times \{\exp[-(a_1 r_{12} + a_2 r_{13} + a_3 r_{23})] + \exp[-(b_1 r_{12} + b_2 r_{13} + b_3 r_{23})]\} . \quad (5)$$

r_{ij} are interparticle distances. The wave function is normalized as $\int |\psi_S|^2 d^3\rho\, d^3 r = 1$. The fusion rate is proportional to the fusion integral I_f, where

$$I_f = \lim_{\rho \to 0} \int d^3 r\, |\psi(\mathbf{r},\rho)|^2 . \quad (6)$$

The following cusp constraints are imposed on the variational parameters to remove the singularities at $r_{12} = 0$ and $r_{12} = r_{13} = r_{23} = 0$,

$$\lim_{r_{12} \to 0} \left(\frac{1}{\psi_S} \frac{\partial \psi_S}{\partial r_{12}} \right) = \frac{m_1 m_2}{m_3 (m_1 + m_2)} = d_1 , \quad (7)$$

$$\lim_{r_{13}, r_{23} \to 0} \left(\frac{1}{\psi_S} \frac{\partial \psi_S}{\partial r_{13}} \right) = -\frac{m_1}{m_1 + m_3} = d_2 , \quad (8)$$

$$\lim_{r_{23}, r_{13} \to 0} \left(\frac{1}{\psi_S} \frac{\partial \psi_S}{\partial r_{23}} \right) = -\frac{m_2}{m_2 + m_3} = d_3 . \quad (9)$$

Equation (7) is exactly satisfied by requiring $a_2 + a_3 = b_2 + b_3$ (or $a_1 = b_1$) and $C_{(1 n_2 n_3)} = C_{(0 n_2 n_3)} [d_1 + (a_1 + b_1)/2]$. Equations (8) and (9) are exactly satisfied at the point $r_{12} = r_{13} = r_{23} = 0$, by requiring $a_2 + b_2 = -2d_2$, $a_3 + b_3 = -2d_3$, and $C_{(n_1 n_2 n_3)} = 0$, whenever n_2 or n_3 is equal to 1.

(b) *P state.* The P-state wave function is

$$\psi_P = f_1 \rho + f_2 \mathbf{r}', \quad \rho = \mathbf{R}_2 - \mathbf{R}_1 ,$$
$$\mathbf{r}' = \left(\frac{m_1 m_3}{M m_2} \right)^{1/2} (\mathbf{R}_3 - \mathbf{R}_1) + \left(\frac{m_2 m_3}{M m_1} \right)^{1/2} (\mathbf{R}_3 - \mathbf{R}_2) . \quad (10)$$

ρ and $\mathbf{r}'$ are the Jacobian vectors defined in Ref. 6. They span the three-body space with $l = 1$. f_1 and f_2 have the same expansion structure as is in Eq. (5), with different variational parameters. The wave function is normalized as $\int |\psi_P|^2 d^3 r\, d^3\rho = 1$, with ρ and $\mathbf{r}$ as defined in (a). The cusp constraints are

$$\lim_{r_{12} \to 0} \left(\frac{1}{f_1} \frac{\partial f_1}{\partial r_{12}} \right) = \frac{d_1}{2}, \quad \lim_{r_{13}, r_{23} \to 0} \left(\frac{1}{f_1} \frac{\partial f_1}{\partial r_{13}} \right) = d_2 ,$$

$$\lim_{r_{13}, r_{23} \to 0} \left(\frac{1}{f_1} \frac{\partial f_1}{\partial r_{23}} \right) = d_3, \quad \lim_{r_{12} \to 0} \left(\frac{1}{f_2} \frac{\partial f_2}{\partial r_{12}} \right) = d_1 ,$$

$$\lim_{r_{13}, r_{23} \to 0} \left(\frac{1}{f_2} \frac{\partial f_2}{\partial r_{13}} \right) = d_4 = -1 \Big/ \left(\frac{m_1 + m_3}{m_1} + \frac{M}{m_1 + m_2} \right) ,$$

$$\lim_{r_{13}, r_{23} \to 0} \left(\frac{1}{f_2} \frac{\partial f_2}{\partial r_{23}} \right) = d_5 = -1 \Big/ \left(\frac{m_2 + m_3}{m_2} + \frac{M}{m_1 + m_2} \right) .$$

d_1, d_2, and d_3 are defined in (a). The cusp constraints are obtained by taking the appropriate limits of the wave equation (4) in Ref. 6.

If fusion takes place while the two nuclei are in the relative P state, the sticking probability ω_1 and the fusion integral $\bar{I}_{f_1}$ are given by

$$\omega_1 = \frac{1}{\bar{I}_{f_1}} \frac{1}{V_0} \int_{\rho_0} d^3\rho \left| \int f_1 \rho \phi_f(r) d^3 r \right|^2 , \quad (11)$$

$$\bar{I}_{f_1} = \frac{1}{V_0} \int_{\rho_0} d^3\rho \int f_1^2 \rho^2 d^3 r . \quad (12)$$

The outer integral in Eqs. (11) and (12) is limited to a spherical volume V_0 of radius ρ_0. ρ_0 is taken to be 7 fm, the approximate range of nuclear influence. In order to compare with previous fusion rates,[8] the fusion integral is also evaluated:

$$I_{f_1} = \lim_{\rho \to 0} \int |\nabla_\rho \psi_P(\mathbf{r},\rho)|^2 d^3 r . \quad (13)$$

The corresponding fusion rates are

$$\bar{\lambda}_1 = \bar{A}_P \bar{I}_{f_1} = (3.6 \times 10^{15} a_n^3/\mathrm{sec}) \bar{I}_{f_1} , \quad (14)$$

$$\lambda_1 = A_P I_{f_1} = (1.1 \times 10^{12} a_n^5/\mathrm{sec}) I_{f_1} . \quad (15)$$

a_n is the muon Bohr radius with infinite nuclear mass, and $\bar{A}_P = v \sigma_P / C_P$. All numbers are taken from Refs. 3 and 8 except C_P. C_P is the P-wave penetration probability defined in Ref. 9 and evaluated at the radial distance 7 fm.

If fusion takes place while the two nuclei are in the relative S state, Eq. (1) can be used to calculate the sticking amplitude, while $\phi_i(\mathbf{r})$ in Eq. (2) is

$$\phi_i(\mathbf{r}) = \frac{1}{\sqrt{I_{f_2}}} \lim_{\rho \to 0} \psi_P(\mathbf{r},\rho) = \frac{1}{\sqrt{I_{f_2}}} \lim_{r_{12} \to 0} f_2 \mathbf{r}' = \frac{C_m}{\sqrt{I_{f_2}}} F_2(r) \mathbf{r},$$
$$C_m = \left(\frac{m_1 m_3}{M m_2} \right)^{1/2} + \left(\frac{m_2 m_3}{M m_1} \right)^{1/2} . \quad (16)$$

In this limit, $\mathbf{r}$ is the distance between the muon and the center of mass of the ^{5}He compound nucleus. The fusion integral I_{f_2} and the fusion rates λ_2 are

$$I_{f_2} = C_m^2 \lim_{r_{12} \to 0} \int f_2^2 r^2 d^3 r , \quad (17)$$

$$\lambda_2 = (8.0 \times 10^{17} a_n^3/\mathrm{sec}) I_{f_2} . \quad (18)$$

Since $\phi_i(\mathbf{r})$ is a P state, Eq. (4) cannot be used to calculate the sticking probabilities. To simplify vector-coupling algebra, we use the wave function

$$\bar{\phi}_i(\mathbf{r}) = U \phi_i(\mathbf{r}) = \frac{C_m}{\sqrt{I_{f_2}}} F_2(r) r \sqrt{4\pi/3} \begin{pmatrix} Y_{11}(\Omega) \\ Y_{10}(\Omega) \\ Y_{1,-1}(\Omega) \end{pmatrix} ,$$

where $U^\dagger U = 1$. U is a unitary transformation matrix.[10] For a transition to the $\mu\,^4$He atomic state $R_{nl}(r) Y_{lm}(\Omega)$, the sticking amplitude is

$$A_{ij} = \sum_{L=0}^{\infty} i^L \sqrt{4\pi} (2L+1)^{1/2} \iint \bar{\phi}_i(r) j_L(Qr) R_{nl}(r) \times Y_{L0}(\Omega) Y_{lm}^*(\Omega) r^2 dr\, d\Omega .$$

The total transition probability from the initial state $\bar{\phi}_i(\mathbf{r})$

TABLE I. Sticking probabilities ω_{nl} in percentage for the ground S state.

nl	ω_{nl} Present work	Ref. 3	Ref. 4
1s	0.6932	0.689	0.6502
2s	0.0992	0.099	0.0934
2p	0.0241	0.024	0.0238
3s	0.0302	0.030	0.0284
3p	0.0087	0.009	0.0086
3d	...	...	0.0003
4s	0.0128	0.013	0.0121
4p	0.0039	...	0.0037
5s	0.0066	...	...
All others	0.018	0.031	0.0244
Total ω_s	0.897	0.895	0.845

to all final states with $l \leq 1$ and total quantum number n can be grouped into the expression

$$W_n = \frac{4\pi C_m^2}{I_{f_2}} (|I_1|^2 + |I_2|^2 + 2|I_3|^2) ,$$

$$I_1 = \int F_2(r) j_1(Qr) R_{n0}(r) r^3 dr ,$$

$$I_2 = \int F_2(r) j_0(Qr) R_{n1}(r) r^3 dr ,$$

$$I_3 = \int F_2(r) j_2(Qr) R_{n1}(r) r^3 dr ,$$

and the sticking probability $\omega_2 = \sum_{n=1}^{5} W_n$.

In Table I, we compare the results of the 500-term ground S state sticking coefficient with those of Refs. 3 and 4. We have quantitative agreement. Table II lists the fusion rates, total sticking probabilities, and the energies of the ground S state using wave functions ranging from 450 to 500 terms. Table III lists the contributions to the total normalization from different parts of the wave function in Eq. (10). These quantities change very little among the converged wave functions. One notices that even though the probability to find the system in f_1 is very large, the contribution to fusion from this part of the wave function is relatively small. In f_1, the nuclei are in the relative P state, the wave function vanishes at the point of coalescence ($\rho = 0$).

In addition to the fusion integral I_{f_1} given by Eq. (13) and Ref. 7, we have calculated $\bar{I}_{f_1}$ given by Eq. (12). The latter allows contribution to the fusion integral from a region determined by the approximate range of the nuclear force (7 fm). The corresponding fusion rates λ_1 and $\bar{\lambda}_1$ are listed in Table IV for comparison. The sticking probability ω_1 calculated from Eq. (11) is very similar to that of the ground S state given in Table II. This is because the initial muon states are S states in both cases, and under the present approximation, the final states are also the same.

TABLE II. Ground S state energy, sticking probabilities and fusion rates calculated with wave functions ranging from 450 to 500 terms.

No. of terms	Energy in eV	ω_s in percentage	Fusion rates $\lambda_s = A_s I_f$
450	−319.13382	0.903	0.70×10^{12} sec^{-1}
460	−319.13389	0.899	0.72×10^{12} sec^{-1}
480	−319.13416	0.902	0.71×10^{12} sec^{-1}
490	−319.13417	0.897	0.70×10^{12} sec^{-1}
500	−319.13419	0.897	0.71×10^{12} sec^{-1}

Even though the probability to find the system in f_2 is very small, the fusion rate λ_2 from Eq. (18) is relatively large. In f_2, the two nuclei are in the relative S state. However, the sticking probability ω_2 is only 0.25% which is less than a third of ω_1(0.88%). This is due to the P-state characteristics of the initial muon in Eq. (16). A calculation has also been carried out using Eqs. (11) and (12) for f_2. We found very little change in ω_2, but a substantial change in the fusion rate which is listed in Table IV under $\bar{\lambda}_2$. The fusion rate λ_2 agrees with the corresponding quantity given in Ref. 4. λ_1 is 20% larger than theirs.

Based on ω_1, ω_2, and $\bar{\lambda}_1$ and $\bar{\lambda}_2$ an overall effective sticking probability of 0.31% for the $J=1$, $v=0$ state can be estimated. If λ_1 and λ_2 were used the value would be 0.38%. The former was obtained with $\rho_0 = 7$ fm. The latter was obtained using the traditional approximation. Using different ρ_0 does not significantly effect the sticking probabilities even though the fusion rates change with ρ_0. Table IV summarizes the results for the $J=1$, $v=0$ state, using five variational wave functions ranging from 692 to 740 terms. In all cases, equal number of terms are used in f_1 and f_2.

The S state results agree with previous calculations using other methods. The P state has two very different sticking probabilities and fusion rates depending on the initial configurations of the nuclei before fusion, from which an overall effective muon-sticking probability of 0.31% is obtained for $J=1$, $v=0$ state.

It is shown that the variational method is capable of high-precision calculations for the muon molecular three-body systems. Such calculations will open the door to a more realistic treatment of the sticking probability and the fusion rate in the future.

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TABLE III. Normalization constants of our 740-term P-state wave function.

$\int f_1^2\rho^2 d^3\rho d^3r$	$2\int (f_1\rho\cdot\mathbf{r}f_2) d^3\rho d^3r$	$\int f_2^2 r^2 d^3\rho d^3r$
0.979460327642412	0.020260586479703	0.000279085877885

TABLE IV. $J=1$, $v=0$ state energy, sticking probabilities, and fusion rates calculated with wave functions ranging from 692 to 740 terms.

No. of terms	Energy in eV	Sticking probability in percentage		Fusion rates per sec			
		ω_1	ω_2	$\bar{\lambda}_1$	λ_1	λ_2	$\bar{\lambda}_2$
692	−232.468 59	0.872	0.261	1.6×10^7	2.5×10^7	1.0×10^8	1.6×10^8
704	−232.468 60	0.859	0.251	1.6×10^7	2.5×10^7	1.0×10^8	1.6×10^8
716	−232.468 62	0.876	0.250	1.6×10^7	2.5×10^7	1.0×10^8	1.7×10^8
728	−232.468 66	0.904	0.259	1.6×10^7	2.5×10^7	1.0×10^8	1.6×10^8
740	−232.468 67	0.884	0.243	1.6×10^7	2.5×10^7	1.0×10^8	1.7×10^8

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