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Variational calculations of the excited-state fusion parameters of the $(dt\mu)$ system

Chi-yu Hu
Department of Physics, California State University, Long Beach, California 90840
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The energies, muon–alpha-particle sticking probabilities, and the fusion rates have been calculated for the $J=0$, $\nu=1$ and the $J=1$, $\nu=1$ states of the $(dt\mu)$ system. The results for the $J=0$, $\nu=1$ state generally agree with previous calculations using the adiabatic representation basis. The muon–alpha-particle sticking probability is obtained for the $J=1$, $\nu=1$ state for the first time. A small muon–alpha-particle sticking probability obtained for this state raises interesting possibilities for muon-catalyzed fusion.

I. INTRODUCTION

Both the sticking probability and the fusion rate of the $J=0$, $\nu=1$ state have been calculated previously using an elaborate adiabatic representation basis.[1,2] No previous calculation of the sticking probability of the $J=1$, $\nu=1$ state has been reported.

The weakly bound excited P state ($J=1$, $\nu=1$) of the $(dt\mu)$ system is considered to be the gateway of $(dt\mu)$ muon-catalyzed fusion. It has a large resonance formation rate.[3,4] Theoretical study of this state is difficult due to its loosely bound structure. Until recently, it was generally considered impossible by many experts to calculate properties from this state using the variational method. This variational calculation gives a μ-sticking probability and fusion rate of the $J=0$, $\nu=1$ state comparable with that given by previous calculation.[1,2] The variational energy obtained for the $J=1$, $\nu=1$ state is well converged. As a result, it is possible to give meaningful calculation for the μ-sticking probability of this state.

The structure of the variational wave functions are described in Sec. II. Results of the calculation are presented in Sec. III. Sensitivity of the results to the nonlinear variational parameters will be investigated here also. Some speculation in light of the present calculation will be given in Sec. IV.

All the present calculations of the fusion rates and the μ-α sticking probabilities are still based on the sudden approximation described previously in Ref. 5. The variational method is given in Ref. 6. All non-Coulomb interactions and relativistic corrections are neglected at the present time.

II. THE STRUCTURE OF THE VARIATIONAL WAVE FUNCTION

For the excited S state ($J=0$, $\nu=1$) we have

$$\begin{aligned}\Psi=&\sum_{n_1}\sum_{n_2}\sum_{n_3} C_{n_1n_2n_3} r_{12}^{n_1}(r_{13}^{n_2}r_{23}^{n_3}+r_{13}^{n_3}r_{23}^{n_2})\{\exp[-(a_1r_{12}+a_2r_{13}+a_3r_{23})]+\exp[-(b_1r_{12}+b_2r_{13}+b_3r_{23})]\}\\&+\sum_{n_1}\sum_{\substack{n_2\\(n_2\neq n_3)}}\sum_{n_3} D_{n_1n_2n_3} r_{12}^{n_1}(r_{13}^{n_2}r_{23}^{n_3}-r_{13}^{n_3}r_{23}^{n_2})\{\exp[-(e_1r_{12}+e_2r_{13}+e_3r_{23})]+\exp[-(g_1r_{12}+g_2r_{13}+g_3r_{23})]\}\ .\end{aligned} \tag{1}$$

TABLE I. Nonlinear variational parameters used in the S states. The units are the inverse muon Bohr radius.

	a_1	a_2	a_3	b_1	b_2	b_3	e_1	e_2	e_3	g_1	g_2	g_3
$J=0$, $=1$	0.93	1.201	0.73	0.93	0.726	1.163	0.757	0.975	0.39	1.09	0.491	1.221

TABLE II. Nonlinear variational parameters used in the excited P state ($J=1$, $\mu=1$) in units of muon Bohr radius. Those in the first and second rows belong to f_1 and f_2, respectively.

a_1	a_2	a_3	b_1	b_2	b_3	e_1	e_2	e_3	g_1	g_2	g_3
0.777	0.644	0.599	0.777	1.2835	1.2943	0.357	0.957	0.235	0.357	0.425	0.987
0.598	0.75	0.239	0.598	0.2208	0.7231	0.357	1.101	0.255	0.357	0.341	0.981

r_{ij} are interparticle distances. The indexes $i=1,2,3$ refer to triton, deuteron, and muon, respectively. The a's and b's are subjected to cusp constraints. The constraints are described in detail in Ref. 5. The e's and the g's are not required to satisfy the cusp constraints, since this part of the wave function is identically zero at $r_{12}=0$. Some $n_i=1$ terms are excluded to satisfy cusp constraints as $r_{12}=0$ and subsequently $r_{13}=r_{23}\to 0$. The nonlinear parameters used in this calculation for the excited S state are listed in Table I. The variational energies are very sensitive to these nonlinear parameters when the total number of terms in the wave function expansion is small (i.e., less converged). For more converged wave functions, a slight change in them does not significantly affect the binding energies or the sticking probabilities. Details of this investigation will be given in Sec. III.

For the excited P state ($J=1$, $\nu=1$) we have

$$\Psi p=\boldsymbol{\rho} f_1+\mathbf{r} f_2 ,$$

$$\boldsymbol{\rho}=\mathbf{R}_2-\mathbf{R}_1 ,$$

$$\mathbf{r}=\left[\frac{m_1 m_3}{M m_2}\right]^{1/2}(\mathbf{R}_3-\mathbf{R}_1)+\left[\frac{m_2 m_3}{M m_1}\right]^{1/2}(\mathbf{R}_3-\mathbf{R}_2) . \quad (2)$$

The $\mathbf{R}_i$ are the coordinates of the three particles. m_1, m_2, and m_3 are the masses of the triton, deuteron, and muon, respectively, and $M=m_1+m_2+m_3$. $\boldsymbol{\rho}$ and $\mathbf{r}$ are the Jacobian vectors for the three-body systems.[6] f_1 and f_2 both have structure identical to that given in Eq. (1). After satisfying the cusp constraints,[5] there are a total of 18 independent nonlinear variational parameters. They are listed in Table II.

III. RESULTS AND DISCUSSIONS

For easy comparison with other calculations,[7] the masses used are $m_1=5496.918m_e$, $m_2=3670.481m_e$, and $m_3=206.769m_e$. m_e is the electron mass.

The sticking probability for the excited S state is given in Table III. The table lists contributions from various final states of the μ^4He system. These are compared with the corresponding values given in Ref. 1 and listed in column 3.

Even though the present results seem to be 2% higher than those of Ref. 1, an agreement is considered reasonable in light of the uncertainty in the theoretical calculations. The extent of the uncertainty in the present calculation is indicated in Table IV, where the sticking probabilities and fusion rates are given for 10 variational wave functions ranging from 672 terms to 780 terms. Two of them have different nonlinear parameters. The ten wave functions are obtained by successively adding five to ten terms to each of the two series in Eq. (1), in order of increasing $n_1+n_2+n_3$. The maximum value of the n_i is 9 and the maximum $n_1+n_2+n_3=21$.

Table V reports the sticking probability and fusion rate of our more converged $J=0$, $\nu=0$ wave functions. The improvement of the 695-term wave function is partly due to the inclusion of terms with $n_2=1$, $n_3=1$. These terms were excluded from our previously reported 500-term wave function since they do not satisfy the cusp constraints at $r_{13}=0$, $r_{23}=0$. They are included in the 695-term wave function as long as the cusp constraints at $r_{12}=0$ and $r_{13}=r_{23}\to 0$ is satisfied. This improved wave function also gives a sticking probability 4.5% less than that reported previously.[5]

Table VI lists the various components of the excited P state ($J=1$, $\nu=1$). They are compared with the corresponding quantities of the ground P state[5] ($J=1$, $\nu=0$). It is noticed that f_2, the substructure dominated by two nuclei in relative S state, is larger for the excited P state. It is therefore not surprising to find a larger fusion rate for the excited P state as compared with that of the ground P state.[5]

Table VII lists various fusion rates, sticking probabilities, and variational energies for the excited P state obtained with variational wave functions ranging from 1066 to 1102 terms. The previous calculation[2] which reported fusion rates is also listed for comparison. Fusion can take place from both configuration f_1 and f_2, respectively. They have different sticking probabilities and fusion rates.[5] The overall average sticking probability is 0.10%. This value is less than half of that of the ground

TABLE III. Sticking probabilities ω_{nl} in percentage for the S state compared with those in Ref. 1.

n_l	ω_{nl}, $j=0$, $\nu=1$ Present work	Ref. 1
1s	0.6661	0.6526
2s	0.0963	0.0937
2p	0.0238	0.0239
3s	0.0293	0.0285
3p	0.0086	0.0086
3d		0.0003
4s	0.0125	0.0122
4p	0.0039	0.0038
5s	0.0064	
All others	0.018	0.0245
Total ω_s	0.865	0.848

TABLE IV. Excited S-States ($J=0$, $v=1$) energy, sticking probabilities, and fusion rates for ten variational wave functions. For comparison, the fusion rate given in Ref. 2 for this state is 1.0×10^{12} sec^{-1}.

Number of terms	Energy (eV)	ω_s (%)	Fusion rates (sec^{-1})	$(n_1+n_2+n_3)_{\max}$
672	$-34.833\,22$	0.8845	0.59×10^{12}	18
693	$-34.833\,28$	0.8881	0.59×10^{12}	19
707	$-34.833\,29$	0.8786	0.59×10^{12}	19
717	$-34.833\,29$	0.8884	0.59×10^{12}	19
730[a]	$-34.833\,26$	0.8741	0.59×10^{12}	19
730	$-34.833\,30$	0.8710	0.59×10^{12}	19
740[a]	$-34.833\,26$	0.8739	0.59×10^{12}	20
740	$-34.833\,30$	0.8705	0.59×10^{12}	20
760	$-34.833\,30$	0.8717	0.59×10^{12}	21
780	$-34.833\,32$	0.8649	0.60×10^{12}	21

[a]The nonlinear variational parameters used in these wave functions are different with $a_1=b_1=0.905$.

TABLE V. Ground S-state ($J=0$, $v=0$) energy, sticking probabilities, and fusion rates for well-converged variational wave functions. For comparison, the fusion rate given in Ref. 2 for this state is 1.2×10^{12} sec^{-1}.

Number of terms	Energy (eV)	ω_s (%)	Fusion rates (sec^{-1})	$(n_1+n_2+n_3)_{\max}$
647	$-319.140\,10$	0.8591	0.73×10^{12}	18
659	$-319.140\,10$	0.8633	0.73×10^{12}	18
671	$-319.140\,10$	0.8603	0.73×10^{12}	18
683	$-319.140\,10$	0.8581	0.73×10^{12}	19
695	$-319.140\,10$	0.8583	0.73×10^{12}	19

TABLE VI. Normalization constants for the 740-term ground P-state wave function (first row) and for the 1102-term excited P-state wave function (second row).

	$\int f_1^2\rho^2 d^3\rho\, d^3r$	$2\int (f_1\boldsymbol{\rho}\cdot\mathbf{r}f_2)d^3\rho\, d^3r$	$\int f_2^2 r^2 d^3\rho\, d^3r$
$J=1,\ v=0$	0.979 460 327 642 412	0.020 260 586 479 703	0.000 279 085 877 885
$J=1,\ v=1$	0.971 016 584 325 684	0.028 658 553 500 395	0.000 324 862 173 921

TABLE VII. Excited P-state ($J=1$, $v=1$) energy, sticking probabilities, and fusion rates calculated with wave-function range from 1066 to 1102 terms. The subscripts 1 and 2 refer to the configuration f_1 and f_2 in Eq. (2). λ_1,λ_2 are fusion rates obtained using traditional methods. $\bar\lambda_1,\bar\lambda_2$ are fusion rates averaged over a sphere of radius 7 fm^5 around the point of nuclear coalescence. The results give an effective sticking probability $\omega_P=(\bar\lambda_1\omega_1+\bar\lambda_2\omega_2)/(\bar\lambda_1+\bar\lambda_2)=0.10\%$. For comparison, the results of Ref. 2 are also listed. ω_P has an estimated convergence error of $\pm20\%$.

Number of terms for present calculation or reference number for previous calculations	Energy (in eV)	Sticking probability in percentage ω_1	ω_2	Fusion rates per second $\bar\lambda_1$	λ_1	$\bar\lambda_2$	λ_2
1066	$-0.657\,941$	0.4489	0.1069	0.925×10^{7}	1.319×10^{7}	3.036×10^{8}	1.798×10^{8}
1078	$-0.657\,975$	0.4753	0.0809	0.931×10^{7}	1.334×10^{7}	3.008×10^{8}	1.782×10^{8}
1090	$-0.657\,990$	0.4763	0.0825	0.932×10^{7}	1.340×10^{7}	2.865×10^{8}	1.696×10^{8}
1102	$-0.658\,025$	0.4865	0.0836	0.930×10^{7}	1.345×10^{7}	2.944×10^{8}	1.744×10^{8}
Ref. 2	-0.64				1.3×10^{7}		3.9×10^{7}

P state[5] and less than $\frac{1}{8}$ of those of the S states.[1,5,7]

The fusion rate λ_2 is considerably larger than that reported in Ref. 2. This is not surprising since the present wave function is considerably more converged. Table VI shows that f_2 is only a small part of the wave function. It is also more slowly convergent than the wave function as a whole. Since the present wave function is very well converged, the improvement in λ_2 is more noticeable than that in λ_1.

IV. CONCLUSION

Due to the small μ-sticking probability for the $J=1$, $v=1$ state, if there were a significant fraction of fusion taking place in this state, the effective sticking probability could be reduced and the number of fusions per muon could be increased. However, according to calculation based on the sudden approximation, the fusion rate is too small to compete with the cascade processes where the $(dt\mu)$ molecule drops to lower energy levels by ejecting Auger electrons.[2] It is therefore essential for the theorists to carefully reexamine the present approximations and for the experimentists to find ingenious means to enhance the relative population of this critical gateway state.

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