Ground-state $dt\mu$ fusion rate and sticking probability using perimetric coordinates

Benjamin P. Carter
1612 Third Street, Manhattan Beach, California 90266

Chi-yu Hu*
University of California at Los Angeles, Los Angeles, California 90024-1547
(Received 19 July 1989; revised manuscript received 1 March 1990)

The ground-state energy, fusion rate, and sticking probability are calculated using a Laguerre polynomial basis. The results are compared with previous calculations, and the advantages are pointed out.

We report the results of a calculation where a Laguerre polynomial basis similar to that used by Pekeris[1] in helium-atom calculation has been applied to the ground state of the $(dt\mu)^+$ molecular ion. The variational wave function is

$$\phi=\sum_{(N_1,N_2,N_3,)} A(N_1,N_2,N_3) \times \exp[-(\gamma_1 r_1+\gamma_2 r_2+\gamma_3 r_3)] \cdot \times \prod_{i=1}^{3} 2L_{N_i}^{(-1)}(x_i) \quad (1)$$

The N_i's are triplets of non-negative integers. The γ's are nonlinear variational parameters. r_1, r_2, and r_3 are interparticle distances. r_3 is the internuclear distance. r_1 and r_2 are distances between muon, deuteron and muon, triton, respectively. The perimetric coordinates x_i are given by

$$x_i=(\gamma_j+\gamma_k)(r_j+r_k-r_i) , \quad (2)$$

where i, j, and k are distinct integers in the range from 1 to 3. The generalized Laguerre polynomials $L_{N_i}^{(-1)}(x_i)$ used in Eq. (1) lead to a sparse kinetic energy matrix and the Hamiltonian matrix is well behaved, so that very large variational expansion can be used without double-precision computation. We have used nearly 3000 terms. The matrices showed no sign of any ill condition. Extremely accurate sticking probability for the $(dt\mu)^+$ system is obtained very economically.

The masses used are given in Table I. The nonlinear parameters are listed in Table II. The parameters used to determine the number of terms in the variational expansions are given in Table III, so that our wave function can be reproduced easily.

The linear variational parameters $A(N_1,N_2,N_3)$ and the variational energies are obtained using a variational iterative method described in detail in Ref. 2. The sticking probability and fusion rates are obtained using sudden approximation[3] where the $(dt\mu)^+$ wave function at the nuclear coalescence point is given by setting $r_3=0$, $x_1=x_2=0$, and $r_1=r_2=r$. Then Eq. (1) becomes

$$\phi(r)=\sum_{(N_1,N_2,N_3)} 8A(0,0,N_3)L_{N_3}^{(-1)}(x_3) \times \exp[-(\gamma_1+\gamma_2)r] . \quad (3)$$

The normalized wave function for the initial state of the muon (relative to the coalesced nuclei) is

$$\phi_i(r)=\phi(r)\Big/\left[\int 4\pi r^2 dr|\phi(r)|^2\right]^{1/2} . \quad (4)$$

The sticking probability for a transition to a μ^4He atom in the quantum state nl is given by[4,5,6]

$$\omega_{nl}=4\pi(2l+1)\left|\int \phi_i(r)R_{nl}(r)j_l(Qr)r^2 dr\right|^2 . \quad (5)$$

$R_{nl}(r)$ is the radial function of the μ^4He atom, $j_l(Qr)$ is a spherical Bessel function, and $Qa_\mu=5.844$ (Ref. 6) (a_μ is the muon Bohr radius). The Bessel function arises from a partial wave decomposition of the plane wave that represents the relative motion between μ^4He and the ejected neutron after the nuclear reaction. The total sticking probability is

TABLE I. Particle indices and masses.

Index i	Type of particle	Mass ratio[a] m_i/m_e
1	triton	5496.918
2	deuteron	3670.481
3	muon	206.769

[a]Where m_e is the mass of an electron.

TABLE II. Nonlinear parameters in the trial wave function.

Particle indices[a]	Nonlinear parameter[b] [(units of a_μ)$^{-1}$]
1,2	$\gamma_3=0.997$
2,3	$\gamma_1=0.931$
3,1	$\gamma_2=0.981$

[a]These indices refer to the particle listed in Table I.
[b]The trial wave function contains a factor $\exp(-\gamma_i r_i)$ for each inter-particle distance r_i (where r_3 for example is the distance between particles 1 and 2).

TABLE III. Number of basis functions and constraints on the four variational functions used. K_1, K_2, K_3 are the maximum order of the three Laguerre polynomials. $K_{\text{tot}} \geq N_1 + N_2 + N_3$.

Parameters of constraints				Number of
K_1	K_3	K_3	K_{tot}	basis functions
11	10	10	22	1287
12	11	11	24	1652
12	12	12	26	1977
13	12	12	28	2565

$$\omega_s = \sum_{n,l} \omega_{nl} \ . \tag{6}$$

Analytical integration of ω_{nl} is obtained for $l \leq 4$ and $n \leq 30$ for the sake of comparison with previous calculation. The fusion rate $A_s I$ is described in detail in Ref. 7 where

$$A_s = 8.0 \times 10^{17}\ a_\mu^3\ \text{sec}^{-1}\ ,$$
$$I = \int 4\pi r^2 dr |\phi(r)|^2 \ . \tag{7}$$

Table IV summarizes the results of energies, fusion rates, and sticking probabilities obtained using five variational wave functions of Eq. (1) ranging from 1287 to 2565 terms. The energy has been stabilized to 11 digits when the trial wave function has 2000 or more terms. This is more accuracy than is necessary, since the masses are only given to six to seven digits and the Rydberg to eight places. However, a large expansion is necessary for convergence in the sticking probability. It is noted that the fusion rate $0.72 \times 10^{12}\ \text{sec}^{-1}$ obtained in this calculation agrees remarkably well with our previous calculations,[7,8] which used a very different generalized Hylleraas-type basis. The 500-term wave function in Ref. 7 gave a fusion rate of $0.71 \times 10^{12}\ \text{sec}^{-1}$, and the 695-term wave function in Ref. 8 gave the value $0.73 \times 10^{12}\ \text{sec}^{-1}$. It is also noted that the fusion rates and the sticking probability converge much faster in our old basis despite its dependence problem. This is due to the large number of terms that are nonzero at the nuclear coalescence point.

In Table V, the sticking probabilities obtained with the present variational function are compared to similar large-basis results.[9] The latter variational function is also a generalized Hylleraas basis similar to our old basis. But the authors overcame the dependence problem using expensive computation techniques. The present basis does not have the dependence problem. All wave functions

TABLE IV. Results of variational calculations 1 Ry = 13.605 804 eV was used. Sticking probabilities are given for two values of Qa_μ.

Number of terms N	Energy (eV)	Fusion rate ($10^{12}\ \text{sec}^{-1}$)	Total sticking probability[a] ω_s (%) $Qa_\mu = 5.844$	$Qa_\mu = 5.846$
1287	−319.140 125 355	0.720	0.8978	0.8961
1652	−319.140 125 405	0.714	0.8851	0.8834
1977	−319.140 125 434	0.716	0.8841	0.8824
2201	−319.140 125 438	0.717	0.8843	0.8826
2565	−319.140 125 432	0.717	0.8843	0.8826

[a]All sticking calculations have been carried out to $n \leq 30$, $l \leq 4$. All other terms contribute 0.0006%; that is, $\omega_s = \sum_{n=1}^{30} \sum_{l=0}^{\max(n-1,4)} \omega_{nl} + 0.000\,006$.

TABLE V. Muon sticking probabilities compared to previous calculations [ω_{nl}(%)].

nl	Present work[a] $Qa_\mu = 5.846$	Ref. 9 $Qa_\mu = 5.846$	Ref. 10 $Qa_\mu = 5.846$
$1s$	0.6800	0.6826	0.6825
$2s$	0.0975	0.0979	0.0978
$2p$	0.0237	0.0238	0.0238
$3s$	0.0296	0.0297	0.0297
$3p$	0.0085	0.0086	0.0086
$3d$	0.0002	0.0002	0.0002
$4s$	0.0126	0.0127	0.0127
$4p$	0.0038	0.0039	0.0039
$4d + 4f$	0.0001	0.0001	0.0001
$5s$	0.0065	0.0065	0.0065
All others	0.0195[b] + 0.0006[c]	0.0200	0.0200
Total	0.8826	0.8860	0.8859

[a]Results for wave function with $N = 2565$ terms.
[b]Calculated for $n \leq 30$, $l \leq 4$.
[c]Estimated for all $n > 30$, $l > 4$.

are obtained using 14-place single precision in a Cray computer.

The set of input masses used in the present calculation are slightly different from that used in Ref. 9 (different in the seventh place at the most). We used their masses in a 695-term calculation and found that the sticking probability differs only in the seventh place. It is completely negligible compared to the 0.004% difference in ω_s between the two calculations as shown in Table V. We used the same Qa_μ value for the sake of comparison. The value of ω_s is very sensitive to the value of Qa_μ used. This can be seen from the two values of Qa_μ listed in Table IV.

Using his large basis variational wave function, Kamimura[10] also obtained a sticking probability of 0.8859%. It appears that ω_s has converged to at least two significant digits.

Our energy of -319.1401 eV agree with at least three[8,11,12] completely different variational calculations using the same sets of masses. We have shown that the Laguerre polynomial basis provides an efficient and economical precision calculation of the $(dt\mu)^+$ ground-state properties.

One of the authors (C.Y.H.) wishes to express her gratitude for many helpful discussions with Dr. James Cohen, Dr. Berni Alder, Dr. S.-I. Salem, and Dr. C. W. Wong, and for support by the National Science Foundation under Grant No. RII8721929. We also wish to thank the San Diego Supercomputer Center for computer time.

*On leave from California State University, Long Beach, CA.

[1]C. L. Pekeris, Phys. Rev. **112**, 1649 (1958).
[2]C. Y. Hu, Phys. Rev. **167**, 112 (1968).
[3]S. Deser, M. L. Goldberger, K. Baumann, and W. Thirring, Phys. Rev. **96**, 774 (1954).
[4]S. S. Gerstein, T. V. Petrov, L. T. Ponomarev, N. P. Popov, L. P. Presnjakov, and L. N. Somov, Zh. Eksp. Teor. Fiz. **80**, 1990 (1981) [Sov. Phys.—JETP **53**, 872 (1981)].
[5]L. Bracci and G. Fiorentini, Nucl. Phys. A **364**, 383 (1981).
[6]D. Ceperly and B. J. Alder, Phys. Rev. A **31**, 1999 (1985).
[7]C. Y. Hu, Phys. Rev. A **34**, 2536 (1986).
[8]C. Y. Hu, Phys. Rev. A **36**, 4135 (1987).
[9]S. Haywood, *et al.*, Phys. Rev. A **37**, 3393 (1988).
[10]M. Kamimura, in *Muon-Catalyzed Fusion,* Proceedings of the Conference on Muon-Catalyzed Fusion, Sanibel Island, Florida, 1988, AIP Conf. Proc. No. 181, edited by Steven E. Jones, Johann Rafelski, and Hendrik J. Monkhorst (AIP, New York, 1989), p. 330.
[11]S. I. Vinitskii *et al.*, Phys. Lett. B **196**, 272 (1987).
[12]A. M. Fralov and V. D. Efros, J. Phys. B **18**, 1265 (1985).