

## Effect of logarithmic terms on the energy level and wave function of a $dt\mu$ system

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(Received 26 June 1989)

The effect of the logarithmic terms on the ground-state energy level and wave function of a  $dt\mu$  system is investigated. No significant contribution of the logarithmic terms on either the energy level or wave function is found. At the same time, we find the lowest upper bound of the ground-state energy ever obtained by the variational method using the Hylleraas-type trial function and that the corresponding wave function satisfies the cusp condition as  $r_{dt} \rightarrow 0$  automatically to a reasonable accuracy for  $r < 3$  (muonic a.u.), where  $r$  is the distance between the fused  $dt$  nuclear compound and the muon.

### I. INTRODUCTION

Bartlett, Gibbons, and Dunn<sup>1</sup> showed that the  $S$ -state wave function of helium could not be expressed as an ascending power series of the interparticle distances. An expansion incorporating the logarithmic terms of the hyperradius  $R$  into the power series<sup>2</sup> was later shown by Bartlett<sup>3</sup> and Fock<sup>4</sup> to be an exact representation of the wave function at small  $R$ , and thus receives much attention since it is believed that an accurate calculation of certain physical observables depends upon a good representation of the wave function near the origin. Macek<sup>5</sup> showed that the Fock expansion of the two-electron atomic wave function with  $L$ ,  $M$ , and parity as good quantum numbers converges for  $R < 1/2|k|$ , where  $k$  is related to the energy of the system by  $k = \sqrt{2E}$ , justifying its existence in that region from a theoretical point of view. More recently, Morgan<sup>6</sup> was able to prove that the Fock expansion for  $S$  states converges pointwise for all values of  $R$ . As for the numerical calculations of the energy levels, although Hylleraas and Midtdal<sup>7</sup> obtained improved results of the energies for the ground states of helium and some of its isoelectronic ions by incorporating a term  $r_1 r_2 \cos\theta \ln(r_1 + r_2)$  and three other nonconventional terms in a 24-term variational wave function, Hart and Herzberg<sup>8</sup> later repeated their 20-parameter calculation with the additional Hylleraas's four nonconventional terms and observed no appreciable lowering of the ground-state energies, leaving the conclusion of Hylleraas and Midtdal unconfirmed. However, both the variational calculations carried out by Ermolaev and Sochilin<sup>9</sup> and by Frankowski and Pekeris<sup>10</sup> give a lower-energy value for the ground state of helium, the former using a standard Fock series as the trial function while the latter including  $[\ln(r_1 + R_2)]^j$  terms for  $j=1$  and 2 in their Hylleraas-type power expansion. Their results therefore seem to support the existence of the logarithmic terms in the exact wave function.

In the investigation of the muon-catalyzed  $dt\mu$  fusion reaction, the theoretical prediction of the muon sticking probability, although improved by the persistent effort of several groups, still deviates significantly from the experimental data available so far. Some example of this are given in Refs. 11–19. Different methods include adiabatic Born-Oppenheimer approximation,<sup>15</sup> numerical treat-

ment of the mesic molecular wave function based on the exact Coulomb three-body adiabatic representation,<sup>16</sup> the Monte Carlo calculation,<sup>17</sup> and the variational technique.<sup>18,19</sup> Generally speaking, while an effective muon sticking probability  $\omega_s$  as low as 0.35% at a target density higher than liquid hydrogen ( $4.25 \times 10^{22}$  atoms/cm<sup>3</sup>) has already been observed,<sup>12</sup> the lowest theoretical prediction of  $\omega_s^0$  (Ref. 20) obtained so far is 0.845%,<sup>16</sup> giving  $\omega_s = 0.541\%$  at a 1.2 liquid hydrogen density by taking into account the muon-stripping process before the mesic-ion ( $\mu\text{-}^4\text{He}^+$ ) is stopped in the hydrogenic isotope medium.<sup>21</sup> The experiments by Breunlich *et al.*<sup>13</sup> and by Nagamine<sup>14</sup> give  $\omega_s = 0.45\%$  and an upper bound 0.44% of  $\omega_s$ , respectively, with no observation of density dependence, which are all lower than the lowest theoretical predictions at either high density, as given above, or low density (0.1 liquid hydrogen density)  $\omega_s = 0.59\%$ . Although the experimental data are still to be improved, the theoretical prediction may not be accurate enough since it depends sensitively on a correct representation of the wave function near the coalescence point, and the wave functions used so far do not exactly satisfy this requirement. This, in turn, naturally leads one to reconsider the effect of logarithmic terms on the ground-state energy and wave function of the  $dt\mu$  system. The present paper is specifically devoted to such a kind of investigation. In Sec. II, we study the basic theory and the analytical calculation. Section III gives the numerical computation of the energy level and muon-sticking probability. Finally, we discuss our results in Sec. IV.

### II. BASIC THEORY

In the center of mass system, a  $dt\mu$  mesomolecular ion has six internal degrees of freedom. The choice of independent variables corresponding to the six degrees of freedom is quite arbitrary, depending on the specific perspective from which the system is going to be described. For example, in the adiabatic Born-Oppenheimer approximation, one may find that it is convenient to use the Jacobian coordinates  $\mathbf{r}_{dt}$  and  $\mathbf{r}_{dt,\mu}$ , where  $\mathbf{r}_{dt}$  connects the deuteron and triton while  $\mathbf{r}_{dt,\mu}$  is the vector displacement of the muon from the center of mass of the deuteron-triton nuclear compound. For the investigation using variational technique, it seems more suitable to choose

three interparticle distance coordinates  $r_{dt}$ ,  $r_{t\mu}$ , and  $r_{d\mu}$ , which define the shape of the triangle with the particles on its vertices and three Euler's angles, which specify the orientation of such triangle in the space. For the  $S$  state, the wave function of the system does not depend on the orientation of the triangle. Therefore the nonrelativistic

Hamiltonian of a  $dt\mu$  system in terms of the interparticle distance coordinates is given by

$$H = T + V, \quad (1)$$

with

$$T = -\frac{1}{2m_{dt}r_{dt}} \frac{\partial^2}{\partial r_{dt}^2} r_{dt} - \frac{1}{2m_{t\mu}r_{t\mu}} \frac{\partial^2}{\partial r_{t\mu}^2} r_{t\mu} - \frac{1}{2m_{d\mu}r_{d\mu}} \frac{\partial^2}{\partial r_{d\mu}^2} r_{d\mu} - \frac{1}{2m_{\mu}r_{d\mu}r_{t\mu}} (-r_{dt}^2 + r_{d\mu}^2 + r_{t\mu}^2) \frac{\partial^2}{\partial r_{d\mu} \partial r_{t\mu}} \\ - \frac{1}{2m_d r_{d\mu} r_{dt}} (r_{dt}^2 + r_{d\mu}^2 - r_{t\mu}^2) \frac{\partial^2}{\partial r_{d\mu} \partial r_{dt}} - \frac{1}{2m_t r_{t\mu} r_{dt}} (r_{dt}^2 - r_{d\mu}^2 + r_{t\mu}^2) \frac{\partial^2}{\partial r_{t\mu} \partial r_{dt}} \quad (2)$$

and

$$V = \frac{1}{r_{dt}} - \frac{1}{r_{d\mu}} - \frac{1}{r_{t\mu}}, \quad (3)$$

where  $m_{ij}$  is the reduced mass of particles  $i$  and  $j$ , and  $r_{ij}$  is the distance between particles  $i$  and  $j$ .

An obvious advantage of the interparticle distance coordinates is their intuitive geometrical significance. However, since the range of one variable depends on the other two due to the triangular condition among them (this statement should not be misunderstood as saying that three interparticle distance coordinates are not independent), one may find difficulties in the analytical calculation of the Hamiltonian matrix elements. For this

reason, we introduce the so-called perimetric coordinates<sup>22</sup> defined in terms of the interparticle distances as

$$x = r_{dt} + r_{d\mu} - r_{t\mu}, \quad (4)$$

$$y = r_{dt} - r_{d\mu} + r_{t\mu}, \quad (5)$$

$$z = -r_{dt} + r_{d\mu} + r_{t\mu}. \quad (6)$$

The linear transformations given by Eqs. (4)–(6) facilitate the analytical calculations involved in this investigation since the ranges of  $x$ ,  $y$ , and  $z$  are from 0 to  $\infty$ . The disadvantage of this transformation is that it makes the Hamiltonian look less compact. In the new coordinate system, the kinetic and potential energies of the  $S$  state become

$$T = -2 \left[ \frac{xy}{m_{\mu}(x+z)(y+z)} + \frac{x(x+y+z)}{m_d(x+z)(x+y)} + \frac{xz}{m_t(x+y)(y+z)} \right] \frac{\partial^2}{\partial x^2} \\ -2 \left[ \frac{xy}{m_{\mu}(x+z)(y+z)} + \frac{yz}{m_d(x+z)(x+y)} + \frac{y(x+y+z)}{m_t(x+y)(y+z)} \right] \frac{\partial^2}{\partial y^2} \\ -2 \left[ \frac{z(x+y+z)}{m_{\mu}(x+z)(y+z)} + \frac{yz}{m_d(x+z)(x+y)} + \frac{xz}{m_t(x+y)(y+z)} \right] \frac{\partial^2}{\partial z^2} \\ + \frac{4xy}{m_{\mu}(x+z)(y+z)} \frac{\partial^2}{\partial x \partial y} + \frac{4xz}{m_t(x+y)(y+z)} \frac{\partial^2}{\partial x \partial z} + \frac{4yz}{m_d(x+z)(x+y)} \frac{\partial^2}{\partial y \partial z} \\ -2 \left[ \frac{1}{m_{dt}(x+y)} - \frac{1}{m_{t\mu}(y+z)} + \frac{1}{m_{d\mu}(x+z)} \right] \frac{\partial}{\partial x} -2 \left[ \frac{1}{m_{dt}(x+y)} + \frac{1}{m_{t\mu}(y+z)} - \frac{1}{m_{d\mu}(x+z)} \right] \frac{\partial}{\partial y} \\ -2 \left[ \frac{-1}{m_{dt}(x+y)} + \frac{1}{m_{t\mu}(y+z)} + \frac{1}{m_{d\mu}(x+z)} \right] \frac{\partial}{\partial z} \quad (7)$$

and

$$V = \frac{2}{x+y} - \frac{2}{x+z} - \frac{2}{y+z}. \quad (8)$$

Correspondingly, we expand the  $S$  wave function of the system in terms of  $x$ ,  $y$ , and  $z$  as

$$\psi_{dt\mu}(x, y, z) = (e^{-ax-by} + e^{-bx-ay}) e^{-cz} \left[ \sum_{n_1, n_2, n_3} A(n_1, n_2, n_3) x^{n_1} y^{n_2} z^{n_3} + \sum_{i, j, k} B(i, j, k) (x^2 \ln x)^i (y^2 \ln y)^j (z^2 \ln z)^k \right], \quad (9)$$

which is later truncated to a finite number of terms. Notice that the first sum in Eq. (9) is just the Hylleraas-type trial function. The matrix element of Hamiltonian can then be calculated analytically with the basis set given by Eq. (9). As the first step, we diagonalize the matrix of the Hamiltonian with all the logarithmic terms in Eq. (9) truncated, and obtain the minimum-energy value of the ground state by varying the nonlinear parameters  $a$ ,  $b$ , and  $c$ . With the corresponding wave function thus obtained, we check the cusp condition as  $r_{dt} \rightarrow 0$  and calculate the muon-sticking probability  $\omega_s^0$ . As the second step, we add six logarithmic terms  $x^2 \ln x$ ,  $y^2 \ln y$ ,  $z^2 \ln z$ ,  $x^2 y^2 \ln x \ln y$ ,  $x^2 z^2 \ln x \ln z$ , and  $y^2 z^2 \ln y \ln z$  to the basis function used in the first step. Namely, in the expansion (9), the second sum goes over only those values of the indices  $i$ ,  $j$ , and  $k$  satisfying

$$0 \leq i, j, k \leq 1 \quad (10)$$

and

$$0 \leq i + j + k \leq 2. \quad (11)$$

We then repeat the same calculations as in the first step, keeping the values of  $a$ ,  $b$ , and  $c$  obtained there unchanged. Notice that after including the logarithmic terms in the wave function used in the first step, the nonlinear parameters  $a$ ,  $b$ , and  $c$  obtained there may no longer be optimal. We keep them unchanged in order to investigate the effect of the logarithmic terms. The difference between the two results, if there is any, will thus give us a measure of the effect of the six logarithmic terms.

Before proceeding to the numerical computation, we briefly review the analytical calculation carried out in this investigation. For each given set of nonlinear parameters  $a$ ,  $b$ , and  $c$ , the upper bound of the Hamiltonian expectation value is obtained by varying the linear coefficients  $A(n_1, n_2, n_3)$  and  $B(i, j, k)$  in Eq. (9). This leads us to the following matrix equation:

$$\underline{H} \underline{A} = \varepsilon \underline{S} \underline{A}, \quad (12)$$

where  $\underline{A}$  is a column matrix representing the wave function. Its elements are given by the coefficients  $A(n_1, n_2, n_3)$  and  $B(i, j, k)$  in Eq. (9).  $\underline{S}$  is the matrix of the unit operator that is not diagonal since the basis set in the wave function expansion (9) is not orthonormal. However,  $\underline{S}$  is real and symmetric and we can always find a unitary matrix  $\underline{U}$  which diagonalizes  $\underline{S}$ . If the numerical result of the diagonalization of  $\underline{S}$  is accurate enough, the eigenvalues of  $\underline{S}$  should be positively definite. We can then solve

$$\underline{H}' \underline{C} = \varepsilon \underline{C}, \quad (13)$$

for  $\varepsilon$  by diagonalizing  $\underline{H}'$ , where

$$\underline{H}' = \underline{\Lambda}^{-1/2} \underline{U} \underline{H} \underline{U}^{-1} \underline{\Lambda}^{-1/2}, \quad (14)$$

with

$$\underline{\Lambda} = \underline{U} \underline{S} \underline{U}^{-1}. \quad (15)$$

Notice that  $\underline{H}'$  is, in fact, the Hamiltonian matrix under

the orthonormalized basis set obtained in the diagonalization of  $\underline{S}$  and  $\underline{C}$  is the matrix representation of the wave function under this new orthonormal basis set. The wave function  $\underline{A}$  under the original basis set is then given by

$$\underline{A} = \underline{U}^{-1} \underline{\Lambda}^{-1/2} \underline{C}. \quad (16)$$

In terms of the perimetric coordinates, the cusp condition as  $r_{dt} \rightarrow 0$  takes the form

$$\lim_{r_{dt} \rightarrow 0} \frac{\partial}{\partial r_{dt}} \ln \psi_{dt\mu} = \lim_{x \rightarrow 0, y \rightarrow 0} \left[ \frac{\partial}{\partial x} + \frac{\partial}{\partial y} - \frac{\partial}{\partial z} \right] \times \ln \psi_{dt\mu} = m_{dt}. \quad (17)$$

As for the probability of the muon sticking to the  $\alpha$  particle and forming a hydrogenic ion  $(\mu\text{-}^4\text{He})^+$  in the state  $(nlm)$ , we accept the conventional definition in terms of the sudden perturbation approximation.<sup>23</sup> It is given by<sup>24</sup>

$$\omega_{nlm}^0 = \left| \int d\mathbf{r} \psi_{nlm}^f(\mathbf{r}) e^{-iq \cdot \mathbf{r}} \psi^i(\mathbf{r}) \right|^2, \quad (18)$$

where  $\psi_{nlm}^f(\mathbf{r})$  is the hydrogenic-type wave function of the mesic-ion  $(\mu\text{-}^4\text{He})^+$  in the state  $(nlm)$ ;  $e^{-iq \cdot \mathbf{r}}$  comes from the recoiling of the ion  $(\mu\text{-}^4\text{He})^+$  due to the sudden emission of the neutron and

$$\psi^i(\mathbf{r}) = \frac{\psi_{dt\mu}(0, 0, z)}{\int |\psi_{dt\mu}(0, 0, z)|^2 d\mathbf{r}}. \quad (19)$$

Notice that in Eq. (19),

$$z = 2r, \quad \text{as } x \rightarrow 0, y \rightarrow 0. \quad (20)$$

For the  $S$  state,  $\psi^i$  does not depend on the angular variables. Therefore, by using

$$\psi_{nlm}^f(\mathbf{r}) = R_{nl}(r) Y_{lm}(\theta, \phi), \quad (21)$$

with  $R_{nl}(r)$  the hydrogenic radial wave function and  $Y_{lm}(\theta, \phi)$  the spherical harmonics, and the partial-wave expansion of  $e^{iq \cdot \mathbf{r}}$  with  $\mathbf{q}$  along the  $\hat{z}$  axis

$$e^{iq \cdot \mathbf{r}} = \sum_{l=0}^{\infty} \sqrt{4\pi(2l+1)} i^l j_l(qr) Y_{l0}(\theta, \phi), \quad (22)$$

Eq. (18) can be reduced to

$$\omega_{nlm}^0 = 4\pi(2l+1) \left| \int r^2 dr R_{nl}(r) j_l(qr) \psi_{dt\mu}(0, 0, 2r) \right|^2 \delta_{m0}, \quad (23)$$

where  $\delta_{m0}$  is just the ordinary Kronecker  $\delta$  function. Notice that in the spherical coordinate system we have chosen here ( $\mathbf{q}$  along the  $\hat{z}$  axis), the muon does not stick to the state  $(nlm)$  with  $m \neq 0$ . Hence the probability of the muon sticking to the state  $(nl)$  is simply given by

$$\omega_{nl}^0 = \sum_{m=-l}^l \omega_{nlm}^0 = 4\pi(2l+1) \left| \int r^2 dr R_{nl}(r) j_l(qr) \psi_{dt\mu}(0, 0, 2r) \right|^2 \quad (24)$$

and the total muon-sticking probability  $\omega_s^0$  is obtained by summing  $\omega_{nl}^0$  over all states  $(nl)$ , namely,

$$\omega_s^0 = \sum_{n=1}^{\infty} \sum_{l=0}^{n-1} \omega_{nl}^0. \quad (25)$$

The calculation of  $q$  value plays one of the key points in the calculation of  $\omega_{nl}^0$  based on the fact that  $\omega_{nl}^0$  is very sensitive to  $q$ . Since our main interest in this paper is to investigate the effect of logarithmic terms, we are not going to discuss this any further. In the numerical analysis presented in the next section, the value of  $q$  is calculated using the method given in Ref. 19. Comparison of two results with and without the logarithmic terms is also given in Sec. III.

### III. NUMERICAL RESULTS

All numerical computations are carried out on IBM 3090 in quadrupole decision which assures at least 32 significant digits. Our results are tested against numerical round-off and/or truncation errors by changing the system of units (for example, from muonic atomic units in which  $m_\mu=1$  to electronic atomic units in which  $m_e=1$ ). The change of unit system dramatically changes the magnitude of the nonlinear variational parameters  $a$ ,  $b$ , and  $c$ , and hence changes the relative magnitude of matrix elements. From the numerical point of view, this would cause significantly different round-off and truncation errors if the program is not stable enough. Since the same results are obtained no matter what kind of units are used, we conclude that, up to the number of digits given in this paper, our results are free from any inherent round-off and truncation errors related to the numerical computation. At the same time, in order to compare our result with the previous calculation,<sup>19</sup> the mass parameters and the Rydberg constant we use here are the same as those given in Ref. 19, namely,  $m_d=3670.481$ ,  $m_t=5496.899$ ,  $m_\mu=206.7686$ , and  $\mathcal{R}=13.605\ 804\ 1$ . Also, since the muon atomic units in which  $e=\hbar=m_\mu=1$  are used throughout, the value of  $q$  corresponding to the given mass parameters is equal to 5.846.

Table I gives the energies of the ground state, where  $n_i^{\max}$  is the upper bound of the summation over  $n_i$  in Eq. (9) and  $n^{\max}$  is the maximum possible value of  $n_1+n_2+n_3$ . We get a faster convergence of the ground-state energy than any previous variational calculation. Notice that in Ref. 19, the ground-state energy  $\epsilon_{00}=319.139\ 752\ 163$  was obtained by using a trial wave function expressed as a sum of 1995 terms, which is still higher than our result  $\epsilon_{00}=319.139\ 834\ 93$  with 435-term

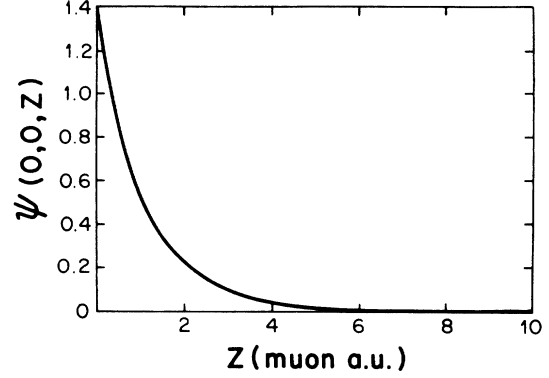


FIG. 1. Comparison of the  $dt\mu$  molecular wave functions with and without logarithmic terms as  $x \rightarrow 0$  and  $y \rightarrow 0$ . On the scale used here, the two curves coincide. (muon a.u. denotes the muonic atomic units in which  $e=\hbar=m_\mu=1$ .)

trial wave function. Since the new coordinates  $x$ ,  $y$ , and  $z$  are simply the linear combination of the interparticle distances, the faster convergence may be attributed to the two-center trial wave function used here as well to the more accurate results of the Hamiltonian matrix elements which are calculated analytically in this paper instead of numerically as in Ref. 19. It should also be pointed out here that although we use two exponential terms in the trial wave function, the number of nonlinear variational parameters are still keep at three, which is the same as used in Ref. 19. Therefore using two exponential terms does not give us any extra flexibility to adjust the wave function to obtain lower ground-state energy level.

From Table I, we also see that the effect of the six logarithmic terms on the energy levels decreases as the number of power terms increases. In fact, as we have already known,

$$\ln x = (x-1) - \frac{1}{2}(x-1)^2 + \frac{1}{3}(x-1)^3 \cdots, \quad \text{for } 0 < x \leq 2 \quad (26)$$

which means that, for  $x$  near unity, the logarithmic term behaves simply as a certain combination of the power terms. Therefore, once the power series expansion converges, the inclusion of the logarithmic terms, which introduce in this case only the effects equivalent to those of the higher power terms, will not change the energy levels significantly. As for the effects of the logarithmic terms on the wave functions, the almost identical results (see Fig. 1) of the 435-term wave function (without log terms)

TABLE I. Binding energy with respect to the  $(t\mu)$ - $d$  threshold and the muon-sticking probability of the  $(dt\mu)$  ground state  $(0,0)$ . The muon-sticking probability given here is obtained by summing the partial sticking probability up to  $n=30$ . The asterisk denotes the numbers of terms given here are those of the expansions without the inclusion of the logarithmic terms.

Number of terms*	$n_1^{\max}$	$n_2^{\max}$	$n_3^{\max}$	$n^{\max}$	Without log terms		With log terms	
					$\epsilon_{00}$ (eV)	$10^2 \omega_s^0$	$\epsilon_{00}$ (eV)	$10^2 \omega_s^0$
84	6	6	6	6	319.130 910 99	0.216	319.131 720 66	0.223
120	7	7	7	7	319.132 110 57	0.045	319.132 996 74	0.044
200	9	9	5	9	319.139 775 70	0.928	319.139 791 35	0.941
344	11	11	7	11	319.139 832 97	0.888	319.139 834 06	0.893
435	12	12	8	12	319.139 834 93	0.875	319.139 835 06	0.875

TABLE II. Comparison of the partial sticking probabilities obtained in this work using 435-term (without log terms) and 441-term (including the six log terms) trial wave functions with the results in Ref. 19 using 1995 basis functions. In all the cases no cusp condition is imposed on the wave function.

$(n, l)$	Without log terms	$10^2 \omega_{nl}^0$ With log terms	Reference 19
(1,0)	0.675 79	0.676 00	0.6826
(2,0)	0.097 20	0.097 22	0.0979
(2,1)	0.023 51	0.023 38	0.0238
(3,0)	0.029 56	0.029 57	0.0297
(3,1)	0.008 48	0.008 44	0.0086
(3,2)	0.000 22	0.000 22	0.0002
(4,0)	0.012 58	0.012 59	0.0127
(4,1)	0.003 81	0.003 79	0.0039
$\sum_{n=1}^{30} \omega_{nl}^0$	0.875 32	0.875 17	0.8854

and the 441-term wave function (including the six log terms) give us the same conclusion as that for ground-state energy. Table II compares our partial sticking probabilities with earlier theoretical values.

The nonlinear parameters  $a$ ,  $b$ , and  $c$  used depend on the number of terms included in the expansion of the trial wave function. For the ground-state 435-term trial wave function,  $a=1.0115$ ,  $b=1.2095$ , and  $c=0.8900$ . In that case, further variation of  $a$ ,  $b$ , and  $c$  around the given values causes only a small shift (about  $10^{-7}$  eV) in the energy level, revealing the nonsensitivity of the dependence of the energy level on the nonlinear parameters when the number of terms in the trial wave functions are big enough. This conclusion is the same as obtained and analyzed in Ref. 19. On the other hand, we notice that the difference between  $a$  and  $b$  should reflect the difference between the masses of the deuteron and triton. Using Eqs. (4)–(6), we can rewrite the exponential term in the trial wave function as

$$e^{-ax-by-cz} = e^{-\alpha r_{d\mu} - \beta r_{t\mu} - \gamma r_{dt}} \quad (27)$$

with

$$\alpha = a - b + c, \quad (28)$$

$$\beta = -a + b + c, \quad (29)$$

$$\gamma = a + b - c. \quad (30)$$

Therefore, for the ground state, we have  $\alpha=0.6920$ ,  $\beta=1.0880$ , and  $\gamma=1.3310$ . If the wave function has a correct asymptotic form,  $\alpha$  and  $\beta$  should be proportional to the reduced masses  $m_{d\mu}$  and  $m_{t\mu}$ , respectively. Since in the muonic atomic units  $m_{d\mu}=0.9467$  and  $m_{t\mu}=0.9637$ , we see that the values of  $\alpha$  and  $\beta$  obtained do not accurately reflect the difference between the masses of deuteron and triton. The second exponential term with  $\alpha$  and  $\beta$  switched compensates this deficiency and as a result, our trial wave function has a better asymptotic form than the wave function with only one

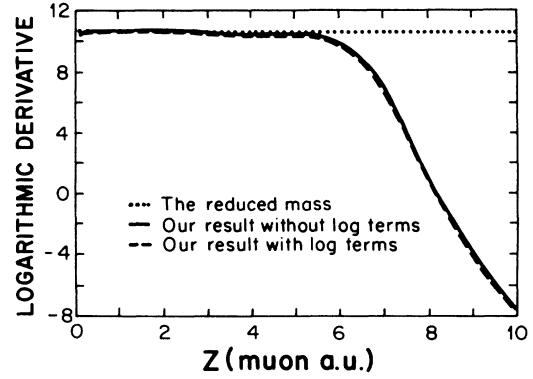


FIG. 2. Logarithmic derivatives with respect to  $r_{dt}$  as  $r_{dt} \rightarrow 0$  of the ground-state wave functions with and without logarithmic terms. See also Eq. (17). (muon a.u. denotes the muonic atomic units in which  $e = \hbar = m_\mu = 1$ .)

exponential term.

The singularity of the first derivative of the logarithmic term at the origin seems to be effectively removed because of its slower speed of divergence than that of the inverse power and hence does not exhibit any influence on the wave function. This is demonstrated numerically in Fig. 2, where we give the logarithmic derivatives with respect to  $r_{dt}$  [see Eq. (17)] of the wave functions in two different cases. It is interesting to notice that for  $z < 6$  (muonic a.u.), two kinds of ground-state wave functions satisfy automatically the cusp condition (17) to a quite

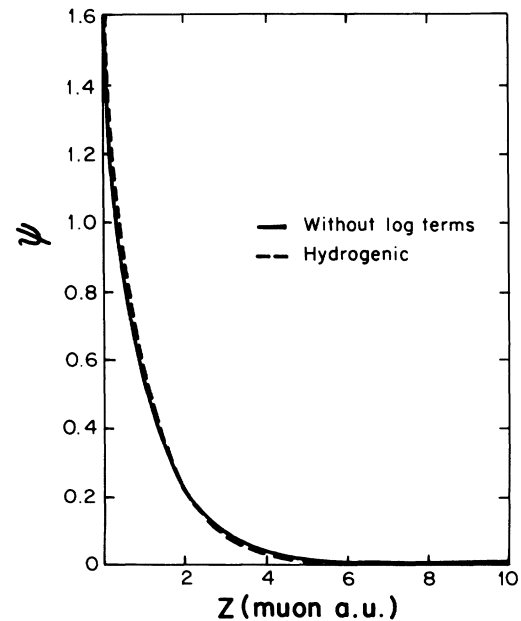


FIG. 3. Comparison of the  $dt\mu$  molecular wave function as  $x \rightarrow 0$  and  $y \rightarrow 0$  with the hydrogenic ground-state wave function of the  $(\mu\text{-}^5\text{He})^+$  ion. (muon a.u. denotes the muonic atomic units in which  $e = \hbar = m_\mu = 1$ .)

reasonable accuracy. Since the wave function is proportional to  $e^{-cz}$  and in this case,

$$e^{-cz} < 0.0048, \quad \text{for } z > 6 \text{ (muonic a. u.)} \quad (31)$$

the deviation of the wave function from the cusp condition for  $z > 6$  should not affect the calculations of the ground-state energy and the corresponding sticking probability significantly. This might explain the similar results obtained in Ref. 19 with and without the cusp conditions imposed on the wave function.

In Fig. 3, we compare the 435-term wave function  $\psi_{dt\mu}(0,0,z)$  (without logarithmic terms) with the exact ground-state wave function of hydrogenic ion  $(\mu\text{-}^5\text{He})^+$ . Two features can be seen there. The first one is that  $\psi_{dt\mu}(0,0,z)$  smears a little more to outer regions than the wave function of  $(\mu\text{-}^5\text{He})^+$ . This means that when the ion  $(\mu\text{-}^5\text{He}^+)$  is formed by the fusion of deuteron and triton in a  $dt\mu$  molecule, the muon is less bound to the nucleus  $(^5\text{He})^{2+}$  than the muon in  $(\mu\text{-}^5\text{He})^+$  in the ground state. The second feature is that the overlap of two functions is almost equal to 1, revealing that the escaping of the muon from the bound state of  $(\mu\text{-}^4\text{He})^+$  when fusion occurs is almost due to the recoil of  $(\mu\text{-}^4\text{He})^+$  as a result of neutron emission.

#### IV. DISCUSSION

In this paper, we study the effect of logarithmic terms on the ground-state energy and wave function of the  $dt\mu$  system and find no significant improvement on either energy or wave function by the introduction of the logarithmic terms. Although  $\ln x$ ,  $\ln y$ , and  $\ln z$  are used instead of  $\ln R$ , where  $R$  is the hyperradius, we notice that  $\ln x$ ,  $\ln y$ , and  $\ln z$  keep the same characteristic of singularity as that of  $\ln R$ , which is the essential point of the Fock expansion theory. Since some lower values of the helium ground-state energy have already been obtained by incorporating the logarithmic terms into the wave function, our result seems to reveal that the effects of the logarithmic terms depend on the mass ratios of the three particles in the system. That is to say, the smaller the mass ratio, the greater the effects of the logarithmic terms. This conclusion is still to be confirmed by further investigation on other three-body systems.

#### ACKNOWLEDGMENTS

I would like to thank Professor J. Macek for useful discussions. Support by the National Science Foundation under Grant No. PHY86-02988 is gratefully acknowledged.

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