Nonvariational calculation of the sticking probability and fusion rate for the μdt molecular ion

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The sticking probability for the μdt molecular ion is estimated with the help of directly calculated nonvariational wave functions obtained by the correlation function hyperspherical harmonic method. The method generates an accurate, locally correct μdt wave function which leads to precise estimates of the partial-wave sticking coefficients and the fusion rate. Our calculations are compared with other precision computations.

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In the past few years the muon-catalyzed fusion reaction

$$dt\mu \xrightarrow{\omega_s^{(0)}} (\alpha\mu + n + \Delta) \qquad dt\mu \xrightarrow{1-\omega_s^{(0)}} (\alpha + \mu + n + \Delta) \tag{1}$$

where $\Delta = 17.6$ MeV is the energy release, has attracted considerable attention. In (1) the sticking coefficient $\omega_s^{(0)}$ is the probability of the first reaction, when the muon in the final state is bound to the α particle. The value of $\omega_s^{(0)}$ plays an essential role in the number of fusion reactions a muon can produce before it decays. This quantity limits the number of synthesis reactions that a muon can catalyze during its lifetime, and thus determines the possibility of using this reaction in energetics.

Calculation of the muon-α-particle sticking coefficient is, therefore, of special importance in muon-catalysis problems. Also, there is an uncertainty in the experimental estimation of this coefficient that makes an accurate theoretical determination of this quantity to be of great significance.

The measured quantity in experiments is not $\omega_s^{(0)}$, but the effective sticking coefficient $\omega_s = (1-R)\omega_s^{(0)}$, where R contains the effect of the stripping, i.e., the reactivation of muons by collisions. Some experimental values [1–3] of ω_s (in %) are 0.45 ± 0.05, 0.35 ± 0.07, and 0.59 ± 0.07; $R = 0.35\pm0.05$ [1,2]. The corresponding estimates of $\omega_s^{(0)}$ (in %) are 0.7 ± 0.13, 0.54 ± 0.15, and 0.91 ± 0.18, respectively. For recent results, see Ref. [4].

In recent years, many different calculations [4–15,17,18,34] of $\omega_s^{(0)}$ were performed that give appreciably larger values of the sticking coefficient. Some values from the literature [4–9] (in %) are 0.8824, 0.886, 0.897, 0.895, 0.845, and 0.858. These theoretical estimates are based on taking into account the Coulomb interaction between the constituents and do not account for corrections due to nuclear interaction in the dt subsystem. These corrections are of the same order of magnitude [4] as the discrepancies in the literature.

The sticking coefficient $\omega_s^{(0)}$ was calculated by many different methods such as adiabatic [17,18], variational [4–6,9–14], and statistical [7] (Green-function Monte Carlo). However, a direct nonvariational approach to the problem using three-body techniques was not yet employed. The purpose of this work is to apply the correlation function hyperspherical harmonic (CFHH) method [19–31] of solving the Schrödinger equation, which is geared to provide not only precise estimates of energy but also wave functions accurate in the whole range of interparticle distances. Use of these wave functions leads in turn to precise estimates of the expectation values of the Hamiltonian and of different operators, including the sticking coefficient.

In the CFHH method [19–31], which is described in Ref. [22], one writes the wave function as a product of two factors,

$$\Psi = \chi\phi \ , \tag{2}$$

where χ is the "correlation factor" and ϕ is expanded in the usual hyperspherical harmonic (HH) functions. If the correlation factor χ is chosen to describe the singular features of Ψ (like cusps) as well as its asymptotic behavior, the function ϕ will be compact, that is, little expanded in space and the HH expansion for it should be rapid. The solution for ϕ proceeds as in the usual HH method, except that the potential V is replaced by an effective velocity-dependent potential V',

$$V' = V - \frac{1}{2}\frac{\nabla^2\chi}{\chi} - (\nabla \ln\chi)\nabla \ , \tag{3}$$

where ∇ is the six-dimensional gradient operator and V is the sum of the interparticle potentials.

In the first CFHH calculation of the μdt system [28], the correlation factor $\chi = \exp(f)$ with a simple linear correlation function

$$f=\sum_{i=1}^{3} b_i r_i \tag{4}$$

was employed. Here b_i are adjustable parameters, chosen to describe the cusp singularities,

$$b_i=\frac{m_j m_k}{m_j+m_k} Z_j Z_k \ , \tag{5}$$

where m_j and Z_j are the mass and the charge of the particle j, and r_i are the interparticle distances in the odd-man-out notation, with $\{d,t,\mu\}$ corresponding to particles $\{1,2,3\}$, respectively. However, such a choice of the parameter b_3, which is positive, leads to wrong asymptotic behavior of the correlation factor. For systems with large $m_1 m_2$, this prevents the CFHH method from converging. Therefore, the linear form (4) forces one to use a different value of this parameter. This corrects the asymptotic behavior of the wave function but destroys the proper description of the dt cusp. The recent more sophisticated μdt calculation [31] employs a nonlinear correlation function

$$f=\sum_{i=1}^{3} [a_i+(b_i-a_i)\exp(-c_i r_i)]r_i \tag{6}$$

geared to reproduce both all the cusps and the asymptotic behavior of the wave function. This guarantees smoothness of the factor ϕ in (2) and correspondingly a fast convergence of the hyperspherical expansion both at small and large interparticle distances r_i. Indeed, at $r_i \to 0$ f has the form

$$f=\sum_{i=1}^{3} [b_i r_i+\mathcal{O}(r_i^2)] \tag{7}$$

so the parameters b_i have to describe the cusp singularities, while at $r_i \to \infty$ f has the form

$$f \approx \sum_{i=1}^{3} a_i r_i \tag{8}$$

and the parameters a_i can be used to provide a proper asymptotic description. Usually a_i are defined by constraints obtained from known cluster asymptotics. Parameters c_i determine the start of the asymptotic region. Use of such a correlation function allows a precise estimate of the wave function for all interparticle distances including the dt coalescence point where the knowledge of the wave function is essential for an accurate calculation of the fusion rate and of the muon sticking probability. In addition, calculation shows [31] that the use of the nonlinear correlation function (6) improves the overall convergence patterns of the expectation values of different operators, including the Hamiltonian, decreasing, for example, the error in energy by an order of magnitude, if the same number of hyperspherical harmonic functions are used. The advantage of the nonlinear correlation function (6) *vis a vis* a linear one is especially obvious from the comparison of Figs. 1 and 2, where values of $H\Psi/E\Psi-1$ (which are identically zero for the exact wave function and whose values at different points characterize, therefore, the extent of the local deviation from the precise wave function) are presented. Note that the scales of Figs. 1 and 2 differ by an order of magnitude.

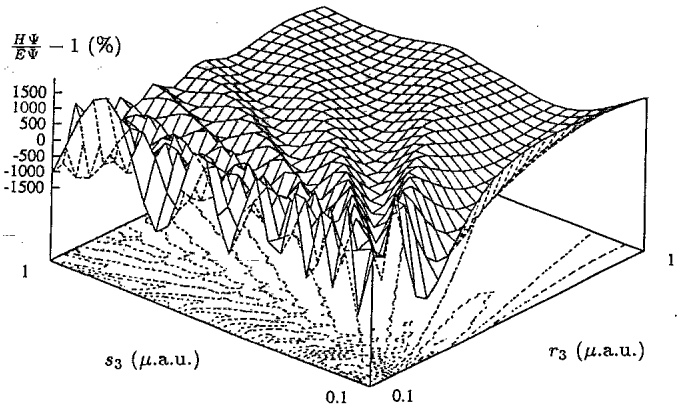

FIG. 1. Values of $H\Psi/E\Psi-1$, in percent, for the linear correlation function f (parametrization A) and $K_m=40$. The coordinate r_3 is the distance between d and t, and s_3 is the distance between μ and the center of mass of d and t. The angle between the corresponding Jacobi vectors is 175° so μ is close to d if r_3 and s_3 have a fixed ratio.

For the present calculation of the sticking probabilities and fusion rates we, therefore, use the wave functions with the nonlinear correlation function f obtained in our work of Ref. [31]. In this work, the following values of the deuteron, triton, and muon masses and of the Rydberg constant ($\mathcal{R}$) most commonly employed in muonic molecules binding energy calculations were used,

$$m_\mu=206.769 m_e, \quad m_d=3670.481 m_e \ ,$$
$$m_t=5496.918 m_e, \quad \mathcal{R}=13.605\,8041 \text{ eV} \ . \tag{9}$$

The choice of parameters a_i, b_i, and c_i is discussed in Ref. [31]. The parameters b_i are given by Eq. (5) while the parameters c_i equal 0.0990, 0.0943, and 0.519

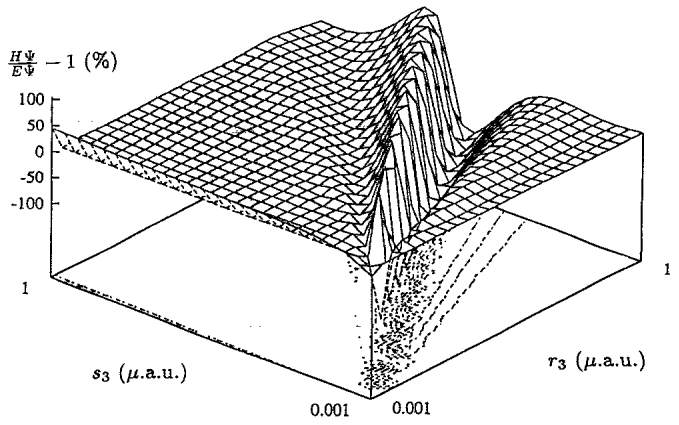

FIG. 2. Same as in Fig. 1, but for the nonlinear correlation function (parametrization C). The vertical scale is different from that of Fig. 1.

TABLE I. Correlation function parameters a_i (in d.a.u., deuteronic atomic units, where mass of the deuteron is set to unity) for different parametrizations A, B, C, and D. Each parametrization may be used with different values of c_i. A refers to linear f. B is defined by the constraint that the asymptotic conditions are imposed on $\exp(f)$. C is such that the asymptotic conditions are imposed self-consistently on the full wave function Ψ at $K_m=0$. (This is a simple nonlinear problem that can be solved before the actual calculation.) D refers to choices without constraints.

	a_1	a_2	a_3
A[a]	−0.054 290 772 4	−0.053 328 776 8	−0.281 664 72
B	−0.017 485 511 192 784	−0.012 356 005 126 688	−0.05
C[b]	−0.054 290 772 402 005	−0.053 328 776 812 877	−0.29
D	0.0	0.0	0.0

[a]Listed are the values of b_i, cf. Eq. (4); b_3 differs from the cusp value, 0.599 615 878, as required for the CFHH method to converge.

[b]The value of a_3 is taken approximately equal to the b_3 of A (first entry). In both A and C parametrizations this parameter is defined by the same constraint.

μ.a.u.$^{-1}$ (muonic atomic units where mass of the muon is set to unity) for $i=1$, 2, and 3, respectively. (Only c_3 appears in the parametrization C.) The parameters a_i are presented in Table I.

The sticking probability $\omega_s^{(0)}$ is the sum of the partial sticking probabilities ω_{nl} defined by the equation [7,11]

$$\omega_{nl}=4\pi(2l+1)\left|\int_0^\infty dr\, r^2 R_{nl}(r) j_l(Qr)\psi(r)\right|^2 \qquad (10)$$

in which averaging over the direction of the outgoing neutron and summation over magnetic quantum numbers is performed.

Here $\psi(r)$ is the three-body wave function Ψ at the point where d and t are located on top of each other, normalized so that the integral of $|\psi(r)|^2$ in the muonic coordinate equals unity, $R_{nl}(r)$ is the radial function of muonic helium, $j_l(Qr)$ is the spherical Bessel function, and Q equals 5.844 in the μ.a.u. (although sometimes a slightly different value of $Q=5.846$, obtained from relativistic kinematics, is used [10,11]).

The results of our calculations of the partial ground-state sticking probabilities and their comparison with previous precision computations are presented in Table II. One can see that the values of the sticking probability are very stable and change very little with the increase of K_m. K_m is the maximum global angular momentum and the number of the HH used is $\frac{1}{2}(K_m/2+1)(K_m/2+2)$. The dependence on the parametrization of f is also negligible and is shown in Fig. 3. From comparison of the values for $K_m=40$ and 48 one concludes that the uncer-

TABLE II. Ground-state sticking probabilities ω_{nl} for $Q=5.844$ calculated with the nonlinear correlation function f. Prescriptions B, C, and D give the same values of ω_{nl} to the number of quoted digits. The second line for $K_m=40$ is for $Q=5.846$.

K_m	1s	2s	3s	4s	2p	3p	4p	3d	4d
32	0.6822	0.0978	0.0297	0.0127	0.0238	0.0086	0.0039	0.0002	0.0001
40	0.6820	0.0978	0.0297	0.0127	0.0238	0.0086	0.0038	0.0002	0.0001
	0.6807	0.0976	0.0297	0.0126	0.0237	0.0085			
48	0.6819	0.0978	0.0297	0.0126	0.0238	0.0086	0.0038	0.0002	0.0001
Ref. [6]	0.6932	0.0992	0.0302	0.0128	0.0241	0.0087	0.0039		
Ref. [7]	0.689	0.099	0.030	0.013	0.024	0.009			
Ref. [10][a]	0.6846								
	0.6826	0.0979	0.0297	0.0127	0.0238	0.0086	0.0039	0.0002	
Ref. [11][b]	0.6817								
	0.6800	0.0975	0.0296	0.0126	0.0237	0.0085	0.0038	0.0002	
Ref. [12][c]	0.6842								
	0.6825	0.0978	0.0297	0.0127	0.0238	0.0086	0.0039	0.0002	
Ref. [4][d]	0.6802	0.0975	0.0296	0.0126	0.0237	0.0086	0.0039	0.0002	

[a]$Q=5.8460$ (second line). Authors state that the change of the total sticking fraction if Q is increased to 5.847 is about −0.001. For our value (5.844) the change would be +0.002 (this extrapolation is shown in the first line, giving even larger disagreement with our value).

[b]Authors quote values for $Q=5.846$ (second line). They also compare with values for $Q=5.844$; the latter values are said to be larger by 0.0017 (in our calculation this difference is 0.0013). The first line was obtained by adding 0.0017.

[c]$Q=5.846$ (second line); the first line was obtained by adding 0.0017.

[d]$Q=5.844$. Quoted are the purely Coulombic results corresponding to an R-matrix formulation imposing the nuclear boundary condition.

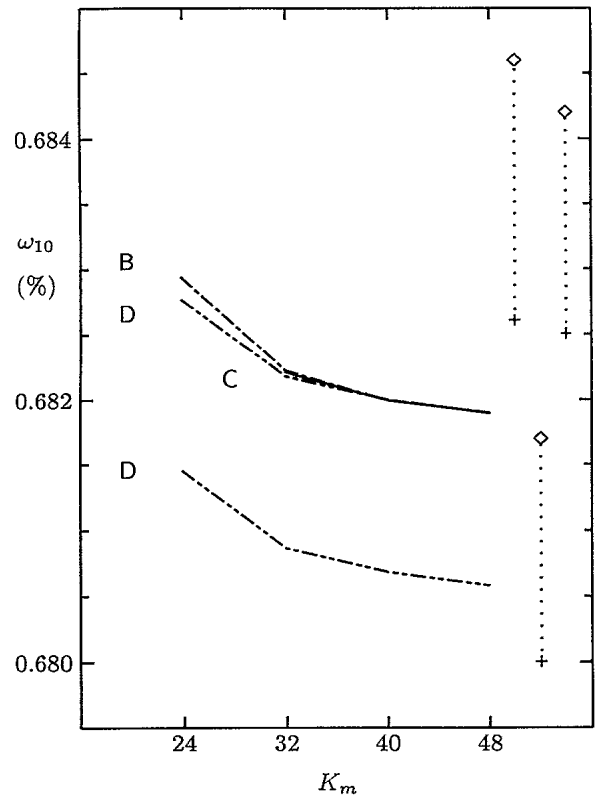

FIG. 3. Ground-state sticking coefficient ω_{10} (in percent) for different parametrizations and its comparison with variational calculations. Upper values correspond to $Q=5.844$ and lower values to $Q=5.846$. Pairs of points on the right are crosses (nonextrapolated variational values) and diamonds (extrapolated variational values). The variational results in sequence from left to right on the graph correspond to Refs. [10, 11, and 12], respectively.

tainty of our $\omega_{10}=0.6819$ value (for $Q=5.844$), for example, is 0.0001 and is less than the differences in the literature for a given value of Q. In particular, the values of Ref. [10] adjusted for Q deviate more from our results than the published values. The recent results of Ref. [4] also deviate appreciably, in the opposite direction.

Table III displays the dependence of the ground-state probability ρ_0 (see Ref. [16]) of the deuteron and triton being together at the same point on K_m (in units of 10^{-13} fm^{-3}). This probability determines the fusion rate [33]: $\lambda_f=A_s\rho_0$. We present ρ_0 rather than λ_f because the convention and value of A_s vary in the literature. The value is [13,32] $A_s=1.3\times10^{-14}$ $\mathrm{cm}^3\,\mathrm{sec}^{-1}$; Ref. [14] uses $\lambda_f=A_r\rho_0$, where $A_r=\frac{3}{2}1.361\times10^{-14}$ $\mathrm{cm}^3\,\mathrm{sec}^{-1}$; Ref. [34] used likewise $\frac{3}{2}A_s=\frac{3}{2}1.36\times10^{-14}$ $\mathrm{cm}^3\,\mathrm{sec}^{-1}$, the factor $\frac{3}{2}$ coming from spin symmetry.

The dependence of ρ_0 on K_m is also shown graphically on Fig. 4. Again, one can see that different parametrizations B, C, and D for the nonlinear correlation function converge to the same value with the increase of K_m and that the uncertainty of our $\rho_0=0.5280\pm0.0011$ value for $K_m=48$ is much less than the discrepancies in the literature.

TABLE III. Probability of d and t being at the same point, $\rho_0=\langle\delta(\mathbf{r}_{dt})\rangle$ (in units of 10^{-13} fm^{-3}), for the ground state of μdt for different parametrizations B, C, and D, and its comparison with variational calculations.

K_m	C	B	D
32	0.5204	0.5250	0.5285
40	0.5250	0.5273	0.5290
48	0.5269	0.5280	0.5287
Ref. [13]		0.5296	
Ref. [14][a]		0.5502	
		0.5294	
Ref. [15][b]		0.594	
Ref. [32][c]		0.6	

[a]Given are fusion rates. We calculated ρ_0 by dividing by the quoted constant, $A_r=2.042\times10^{-14}$ $\mathrm{cm}^3/\mathrm{sec}$. The first line is for the adiabatic case, the second line for the nonadiabatic case.
[b]Misquoted in Ref. [13] as 7.47×10^{-13} (should be divided by 4π).
[c]Extrapolation to nuclear interaction radius zero from Ref. [32], using the quoted coefficient $A_{L=0}=1.3\times10^{-14}$ $\mathrm{cm}^3/\mathrm{sec}$. Reference [32] takes into account the nuclear interaction to estimate ρ_0.

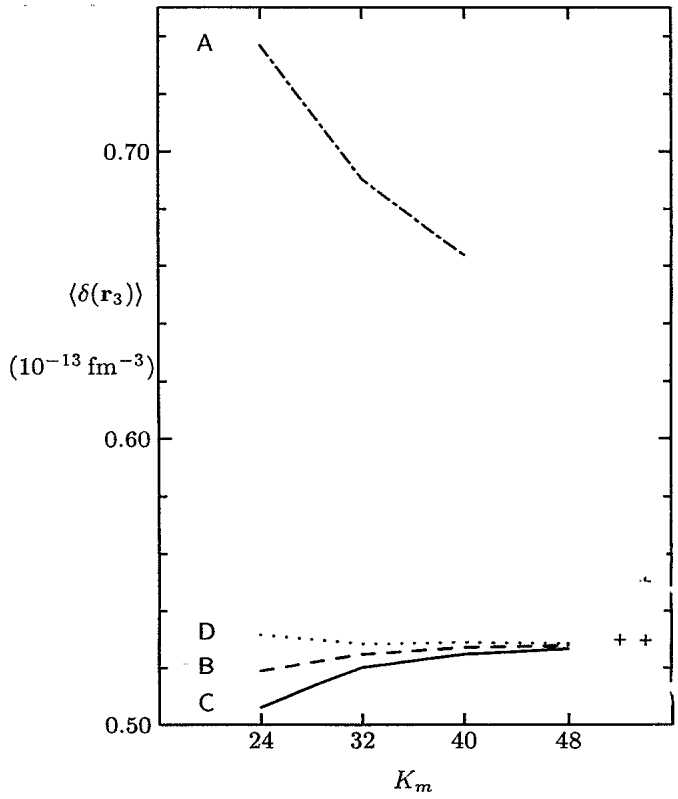

FIG. 4. Expectation values of the δ-function operator of the distance between the deuteron and the triton, proportional to the fusion rate according to the Jackson formula [33], in units of 10^{-13} fm^{-3}, for the linear (parametrization A) and nonlinear (parametrizations B, C, and D) correlation functions. Separate points on the right display the results of variational calculations. The variational results in sequence from left to right on the graph correspond to Refs. [13 and 14], respectively, with the upper (lower) points corresponding to the adiabatic (nonadiabatic) values.

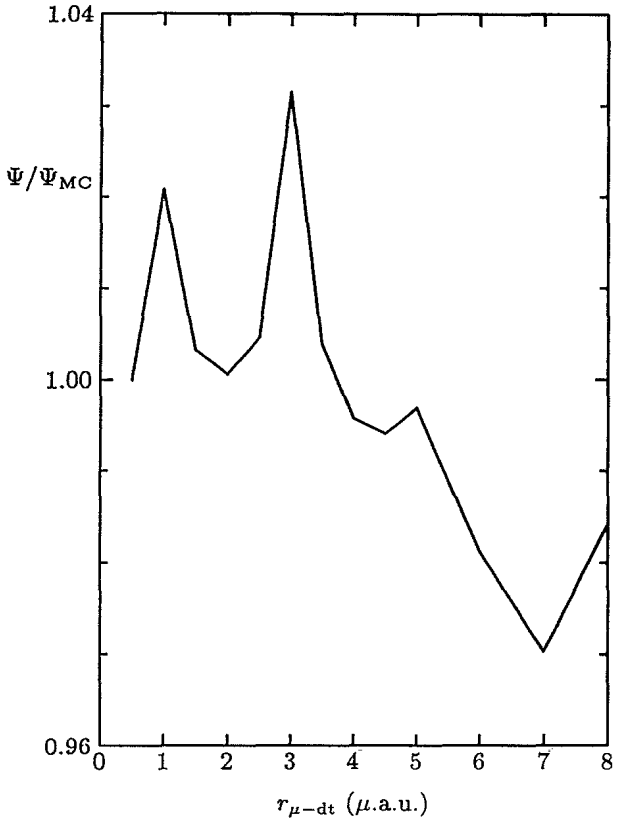

FIG. 5. Ratio of the CFHH wave function Ψ with the nonlinear correlation function (parametrization C, $K_m=40$) at the dt coalescence point (where $\Psi=\psi$) and the Green-function Monte-Carlo wave function Ψ_{MC} of Ceperley and Alder [7]. $r_{\mu-dt}$ is the distance between μ and the center of mass of d and t.

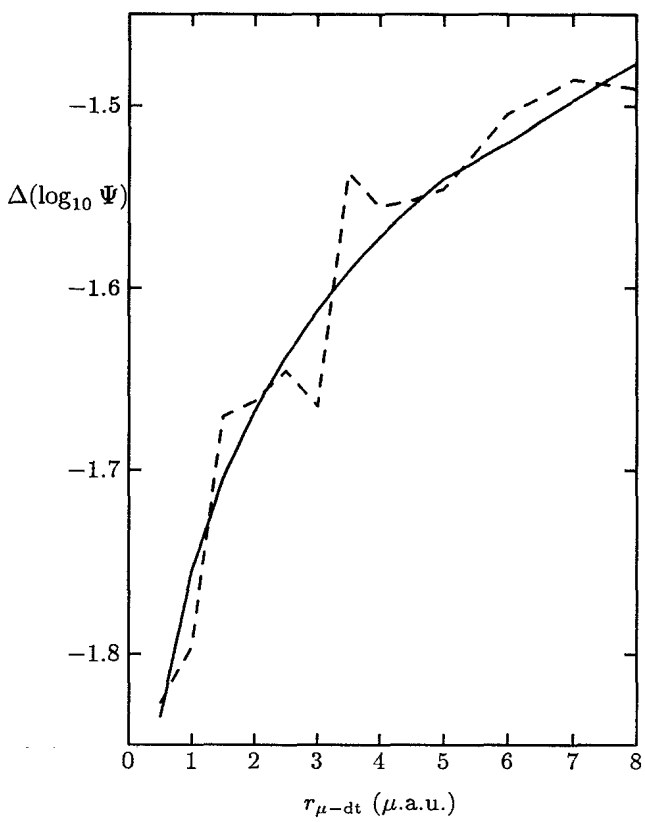

FIG. 6. Divided differences (approximate derivative) of the logarithm of the wave function at the dt coalescence point. The differences correspond to intervals of 0.5 for $r_{\mu-dt}\leq 5$ and to intervals of 1 for $r_{\mu-dt}>5$ (in μ.a.u.). The solid curve is the CFHH wave function calculated with the nonlinear correlation function (parametrization C, $K_m=40$) while the dashed curve represents the Green-function Monte-Carlo wave function of Ceperley and Alder [7]. The Born-Oppenheimer wave function (an exponential) would give a constant value.

It is interesting to compare our wave function with the Green-function Monte-Carlo wave function of Ceperley and Alder [7], which was also used in a nonvariational calculation of the sticking probabilities. The result of the comparison is presented in Figs. 5 and 6, where the ratio of both wave functions and the divided differences of the logarithms of both wave functions at the dt coalescent point are calculated. Figure 5 shows unexpected quasi-periodic deviations from unity. Therefore, we estimated the derivative (Fig. 6) and found that the deviations are caused by the roughness of the Ceperley-Adler wave function.

We have calculated the partial wave sticking probabilities $\omega_{nl}^{(0)}$ and the probability of d and t being at the same point ρ_0 and compared them to values in the literature.

There are significant discrepancies in the literature on the sticking probability and ρ_0 (more so for fusion rates which also depend on the constant A_s adopted), from the point of view of the reliability of various precision computation methods.

Using the CFHH method with a nonlinear correlation function, we have obtained results that have converged much better than discrepancies between different calculations in the literature, both older and recent. Since the expectation values in the CFHH method converge to the correct limits, uncertainty of the results can be deduced from the convergence patterns (Figs. 3 and 4).

No modifications of the method were necessary to get precise wave function at coalescence points; accuracy of the various expectation values is uniform. In variational calculations, it is usually necessary to modify the basis to better describe certain expectation values; frequently, quadruple precision arithmetic has to be used.

The work also confirmed that different parametrizations of the correlation function f give insignificantly different results, as in the case for other expectation values [31]. Also, it is sufficient to use the one parametrization (B) for which the correct cluster asymptotics is imposed on $\exp(f)$. This is the most straightforward of the various prescriptions for choosing the parameters of f (see Table I).

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