Correlation-function hyperspherical-harmonic calculation of the μdt molecular ion

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(Received 8 June 1992)

Direct solution of the Schrödinger equation for the ground and excited S states of the μdt molecular ion is obtained with the help of the correlation-function hyperspherical-harmonic method. Given the proper correlation function, chosen from physical considerations, the method generates wave functions, accurate in the whole range of interparticle distances, which lead in turn to precise estimates of the expectation values of the Hamiltonian and of different functions of interparticle distances. Our results are compared with those obtained in other precision calculations.

PACS number(s): 36.10.Gv

The correlation-function hyperspherical-harmonic (CFHH) method [1–9] of solving the Schrödinger equation for three Coulomb-interacting particles, introduced by Haftel and Mandelzweig a few years ago, has been able to provide together with very precise estimates of energy and of expectation values of different operators also very accurate wave functions.

To date the accuracy of this method has been verified for systems consisting of one heavy and two light particles [2,3,5,7,8], of two heavy and one light particle [6], and of particles of equal masses [4,7,9]. Direct solutions of the Schrödinger equation by the CFHH method for bound three-body atomic systems [1–9] has yielded precision comparable to that obtained previously only by elaborate variational calculations. For maximum global momentum $K_m = 56$, up to nine significant figure precision has been obtained for the energies of the ground and excited states of the helium atom [2,3,5,7,8] and eight significant figures [4,7,9] for the positronium ion $e^- e^- e^+$ (also denoted Ps^-). [The global momentum K in the hyperspherical formalism [1] is an angular momentum in the six-dimensional space defined by the two Jacobi vector coordinates of three particles. Its maximum value K_m determines the number of the basis (hyperspherical harmonic) functions used in a wave-function expansion.] The accuracy of wave functions for the whole range of the interparticle distances and different expectation values for these systems is estimated to be about seven and six significant figures [1–9], respectively.

In recent years interest has accelerated in the three-body muon molecular-ion systems [10–15] (two light ions, e.g., two deuterons, two tritons, or a deuteron and a triton, covalently bonded by a negative muon). This interest stems from the possibility of a fusion reaction (called muon catalyzed fusion or μCF) occurring in the molecule at low temperature and resulting in the liberation of a large amount of energy. This type of reaction requires neither the extremely high temperature nor the huge magnetic fields needed for conventional fusion processes. Hence, muon-catalyzed "cold fusion" (the temperatures needed are of order of 1000 K) could be looked upon as a desirable alternative to conventional fusion [10–15].

Originally the μCF reaction was not regarded as a practical way of generating energy. However, experimental and theoretical advances [10–15] have shown that under the proper conditions a single muon can catalyze about 200 fusion reactions, which is about 40% of the number needed to reach the energy "break-even" point. Future developments in reactor physics, laser excitation, etc., could render μCF practical, and a good understanding of the muomolecules would play a very important role.

The efficiency of μCF depends mainly on the fusion rate and the "sticking probability," i.e., the probability that the muon sticks to a helium nucleus produced in the fusion reaction and is subsequently lost for further catalysis. This will limit how many fusions a single muon (which is expensive to produce) could catalyze. It is important for fusion and sticking-probability calculations to have accurate knowledge of the muomolecular-ion wave function, especially at the so-called "nuclear coalescence point," i.e. where nuclear particles are close together. The fusion rate is determined by the quantum-mechanical probability of tunneling through the Coulomb barrier, as modified by the screening of the negatively charged muon, into the nuclear interaction region. Similarly, the sticking probability also depends on the wave function inside the range of nuclear interaction. However, the usually employed adiabatic approaches [16], which assume

an instant muonic response to nuclear motion, are not precise, since the mass of the muon is not very small compared to the masses of nucleons. Variational wave functions [17–25] are accurate only in the region where the probability density is high, and not necessarily around the nuclear coalescence point (where fusing nuclei are on top of each other), which determines the sticking probability. The Green's-function Monte Carlo method for ground states does not have these limitations, but energies and wave functions obtained by this method are usually not very accurate [26,27]. In addition, its extension to the excited mesomolecular states, which are expected to be the most important in the fusion process, is difficult, due to the fact that any, however, small admixture of the ground state in the important function will eventually dominate the numerical simulation. On the other hand, the wave function obtained by the CFHH method (which is equally applicable to ground and excit-

TABLE I. Calculated ground-state binding energy ε, its expectation value $\langle h \rangle$, and expectation values of different functions of interparticle distances in the odd-man-out notation. The units are eV and muonic atomic units $a_\mu = 2.559\,277 \times 10^{-13}$m, respectively. The parameter b_3 equals -5 except in the second entry for $K_m = 24$ where its value is $-5.680\,512\,6$ (-0.32 in deuteron a.u.). The indices 1,2,3 correspond to deuteron, triton, and muon. K_m is the maximum global angular momentum and N is the number of included hyperspherical functions. The number of digits indicates the numerical precision of calculated values. The variational energies quoted are the best nonextrapolated values.

K_m	N	$\langle r_1^{-2} \rangle$	$\langle r_1^{-1} \rangle$	$\langle \delta(\mathbf{r}_1) \rangle$	$\langle r_1 \rangle$	$\langle r_1^2 \rangle$	ε
24	91	1.234 7	0.758 027	0.175 8	2.032 0	5.451 0	331.859 890
24	91	1.234 3	0.757 80	0.175 76	2.034	5.471	331.756 568
32	153	1.232 283	0.758 262 75	0.175 033 5	2.026 559 6	5.416 081 5	323.010 309
40	231	1.231 434	0.758 214 48	0.174 833 1	2.025 504 2	5.408 838 5	320.753 963
Refs. 23,28,29					2.023		
Refs. 23,25			0.758 3		2.024	5.396	
Ref. 31					2.023	5.397	
K_m	N	$\langle r_2^{-2} \rangle$	$\langle r_2^{-1} \rangle$	$\langle \delta(\mathbf{r}_2) \rangle$	$\langle r_2 \rangle$	$\langle r_2^2 \rangle$	$\langle h \rangle$
24	91	1.124 9	0.721 67	0.155 34	2.128 4	5.949 2	318.408
24	91	1.124 1	0.721 32	0.155 21	2.131	5.969	318.4
32	153	1.122 721	0.721 958 82	0.154 627 2	2.122 905	5.913 54	318.956 9
40	231	1.123 162	0.722 329 5	0.154 670 7	2.120 589 6	5.899 067 6	319.080 203
Refs. 23,28,29					2.117		
Refs. 23,25			0.722 7		2.118	5.882	
Ref. 31					2.118	5.881	
Ref. 19							319.140 10
Ref. 21							319.139 752 161
Ref. 22							319.139 752 161 8
Ref. 23							319.1397
Ref. 24							319.139 606
Ref. 25							319.1411
Ref. 28							319.139 752 161
K_m	N	$\langle r_3^{-2} \rangle$	$\langle r_3^{-1} \rangle$	$10^6 \langle \delta(\mathbf{r}_3) \rangle$	$\langle r_3 \rangle$	$\langle r_3^2 \rangle$	
24	91	0.180 7	0.400 30	1.235 4	2.773	8.441	
24	91	0.180 5	0.399 98	not converged	2.778	8.479	
32	153	0.182 676 9	0.402 467 7	1.157 719 9	2.757 923	8.350 20	
40	231	0.183 270	0.403 135 0	1.112 919 0	2.753 152 5	8.320 714 1	
Refs. 23,28,29					2.747		
Refs. 23,25			0.403		2.748	8.287	
Ref. 31					2.747	8.286	
Ref. 12				12.5[a]			
Ref. 19				0.60			
Ref. 30				0.922 26[b]			
				0.887 37[c]			

[a]A difference by one order of magnitude is believed to be an error due to conversion to cm^{-3}.
[b]Adiabatic.
[c]Nonadiabatic.

ed states [8]) is extremely precise also inside the range of nuclear interaction because the method employs Jastrow correlation functions to exactly account for singularities at coalescence points.

In view of the difficulties of the above-mentioned approaches, and in view of the fact that a first application of the CFHH method to the μpp, μdd, and μtt molecules [6] indeed generated accurate ground-state wave functions for all interparticle distances, including coalescence points, in this paper we extend our study of the CFHH method to the μdt molecular ion, whose properties are of most relevance for muon-catalyzed fusion research [10-15]. We calculate here the ground and excited S states of this system. This is our first test of the method for a system of three nonidentical particles. In this case the number of basis hyperspherical functions describing the system up to a certain precision has to be doubled compared with previously studied systems (He, $e^-e^-e^+$,μpp,μdd,μtt) containing two identical particles, due to the absence of the symmetry requirements which restrict the types of the hyperspherical functions entering a wave-function expansion.

The present calculation is also a prelude to a very accurate investigation of ground and excited S and P states of the μdt molecular ion using a more general nonlinear correlation function f (see below) which is able, for example, to elevate the precision of $e^-e^-e^+$ decay rate computation [9] beyond that reached in the variational approaches.

In the CFHH method we write the wave function as a product of two factors

$$\psi=\chi\phi \ , \tag{1}$$

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 (such as cusps), the HH expansion for ϕ 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'

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

where ∇ is the six-dimensional gradient operator. For the μdt system we employ here a correlation factor $\chi=\exp(f)$ with a simple linear correlation function f:

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

where b_i are adjustable parameters, chosen to describe cusp singularities $[b_i=m_j m_k Z_j Z_k/(m_j+m_k)]$. Here m_j, 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 the completely wrong asymptotic behavior of the correlation factor and therefore we have used a different value of this parameter, given below.

In our calculation the following values of the proton, deuteron, triton, and muon masses and of the Rydberg constant were used:

$$m_\mu=206.769m_e, \quad m_d=3670.481m_e, \quad m_t=5496.918m_e, \quad \mathcal{R}=13.605\,8041 \text{ eV} \ . \tag{4}$$

This set of values is most commonly used in muonic molecules binding energy calculations. In Table I we present the results for the value of parameter $b_3=-5$ which is close to the arithmetic mean of the corresponding values for the μdd and μtt ions (Table III and V of Ref. 6). To show that the results do not depend appreciably on the precise value of b_3, we show in Table I also the results for a different value of b_3.

As one can see from Fig. 1, the convergence pattern of the μdt ground and excited states results is very similar to the pattern of the μdd ground state results of Ref. 6. From the Tables I and II one concludes that our results for the binding energy $\varepsilon=-(E-E_{\mu t})$, where $E_{\mu t}$ is the ground-state energy of the μt atom, the expectation value of binding energy $\langle h\rangle$, $h=-(H-E_{\mu t})$, and for all other expectation values agree with the most sophisticated variational calculations using the Slater-type geminals [21-23] and the generator-coordinate method [25], with the precision of our calculations converged, for example, for the expectation values of the ground-state binding energy up to an error in the fourth significant figure. [As described in our previous work [2], E, the eigenvalue of the effective Schrödinger equation, differs from $\langle H\rangle$, the ex-

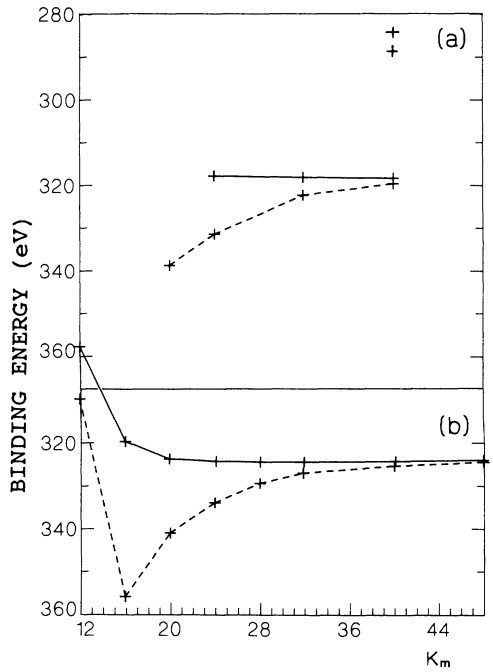

FIG. 1. Binding-energy eigenvalues ε (dashed lines) and their expectation values $\langle h\rangle$ (solid lines), in eV as a function of the maximum global momentum K_m. (a) μdt ground state; the two points near the top correspond to the excited state, the plotted values being $\varepsilon+250$ eV (lower point), and $\langle h\rangle+250$ eV (upper point). (b) μdd ground state, from Ref. 6, for comparison of the convergence patterns.

pectation value of the Hamiltonian, because, with a finite K_m, V' is non-Hermitian. They are both estimates of the energy, but approach each other only for infinite K_m, with $\langle H \rangle$ (not E) having the variational property.]

The general conclusion from the analysis of the results is the applicability of the CFHH method to μdt computations. Improvements in the CFHH method are nevertheless desirable. Indeed, as one can see from Tables I and II, even with 231 hyperspherical functions the inaccuracy of the calculated binding energies is around 0.06 eV for the ground state, and 0.5 eV for the excited state. This inaccuracy is due to the slow convergence with K_m as a consequence of the fact that it is impossible to build in both a satisfactory asymptotic behavior and dt cusp behavior with the linear correlation function f which was previously very successfully used in the computations of the helium atom [2,3,5,7,8] and of the positronium negative ion [4,7]. (Connected with that is also a numerical difficulty [5] in extracting the asymptotic wave function that leads to not being able to obtain precision in expectation values better than the number of significant figures shown in Tables I and II.) In particular, the inability with linear correlation function to include the dt cusp leads to a slow convergence of $\langle \delta(\mathbf{r}_3) \rangle$ which is directly connected with the fusion rate and with the muon sticking probability. For this reason we plan to consider a more general nonlinear correlation function f:

$$f = \sum_{i=1}^{3} [a_i + (b_i - a_i)\exp(-c_i r_i)] r_i \ , \tag{5}$$

geared to reproduce both all the cusps and the asymptotic behavior of the wave function, guaranteeing smoothness of the factor ϕ in (1) and correspondingly a fast convergence of the hyperspherical expansion also at very small and very large interparticle distances r_i. Indeed, at $r_i \to 0$ f has the form

$$f = \sum_{i=1}^{3} b_i r_i \tag{6}$$

TABLE II. As in Table I, but for the excited state.

K_m N	$\langle r_1^{-2} \rangle$	$\langle r_1^{-1} \rangle$	$\langle \delta(\mathbf{r}_1) \rangle$	$\langle r_1 \rangle$	$\langle r_1^2 \rangle$	ε
40 231	1.21	0.707	0.180	2.73	11.6	38.447 072
Refs. 23,28,29				2.738		
Refs. 23,25		0.705 3		2.737	11.74	
Ref. 31				2.738	11.759	
K_m N	$\langle r_2^{-2} \rangle$	$\langle r_2^{-1} \rangle$	$\langle \delta(\mathbf{r}_2) \rangle$	$\langle r_2 \rangle$	$\langle r_2^2 \rangle$	$\langle h \rangle$
40 231	0.763	0.517	0.108	3.89	21.6	34.32
Refs. 23,28,29				3.933		
Refs. 23,25		0.515 4		3.915	22.12	
Ref. 31				3.933	22.395	34.834 465 01
						34.834 464 99
						34.832
Ref. 19						34.833 32
Ref. 21						34.834 465
Ref. 22						34.834 464 7
Ref. 23						34.834 4
Ref. 24						34.834 372[d]
Ref. 25						34.850
Ref. 28						34.834 465
K_m N	$\langle r_3^{-2} \rangle$	$\langle r_3^{-1} \rangle$	$10^6\langle \delta(\mathbf{r}_3) \rangle$	$\langle r_3 \rangle$	$\langle r_3^2 \rangle$	
40 231	0.085 1	0.245	0.933	5.10	30	
Refs. 23,28,29				5.161		
Refs. 23,25		0.244		5.142	30.34	
Refs. 31				5.161	30.629	
Ref. 12			10.4[a]			
Ref. 19			0.49			
Ref. 30			0.799 3[b]			
			0.741 5[c]			

[a]A difference by one order of magnitude is believed to be an error due to conversion to cm^{-3}.
[b]Adiabatic.
[c]Nonadiabatic.
[d]Also written 34.834 327 in the same paper.

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

$$f = \sum_{i=1}^{3} a_i r_i \tag{7}$$

and parameters a_i have to provide a proper asymptotic description. Parameters c_i determine the start of the asymptotic region. Use of such correlation function will allow very precise estimate of 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 the muon sticking probability.

Summing up, the present calculation serves a triple purpose. First, it is a test of our method on a nonsymmetric system which necessitates the doubling of a number of the hyperspherical functions compared with previously considered systems of two identical particles, due to the absence of symmetry requirements. Second, it is a preliminary calculation of μdt which checks the necessity of using the nonlinear generalization of the correlation function able to include all cusps in the wave function without violating the asymptotic conditions. Third, the excited state was calculated in order to be able to compare its precision to the precision of the ground state, and to see improvements due to nonlinear correlation function in future work. In view of these aims, it was not attempted to fine tune the value of the parameter b_3 which has to depart from the cusp value, as described in Ref. 6. Also, the excited state was calculated using the same value of b_3 as used for the ground state, which may not be optimal.

As for results, we have shown that the convergence patterns of the energy eigenvalue, its expectation value and the expectation values of operators depending on interparticle separations, particularly of the δ function operators, are similar to those obtained in the symmetric systems μdd, μtt, etc. (Ref. 6). The same is true for the excited state. In all cases the expectation values of the δ function operators are much more stable than the degree of coincidence between different published values. Nevertheless, the inability to include the cusp condition between the repelling heavy particles if a correlation function linear in interparticle distances is used, limits the accuracy of the calculations. Calculation of the μdt system using a generalized nonlinear correlation function f will be therefore a subject of our future work. In this way the cusp conditions will be satisfied exactly, and the asymptotics of the wave function will be taken into account simultaneously as well. Such a program has recently been carried out successfully for the positronium negative ion [9].

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