Correlation-function hyperspherical harmonic calculations of the $pp\mu$, $dd\mu$, and $tt\mu$ molecular ions

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The direct solution of the Schrödinger equation for the ground state of the $pp\mu$, $dd\mu$, and $tt\mu$ molecular ions 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 leads 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.

The recent experimental observation[1-3] of muon sticking, resulting from the capture of a muon by a ^{3}He or α particle produced in dt or dd muon-catalyzed fusion reactions, calls for a better understanding of this process. This muon-sticking probability ω is of paramount importance since the average number of fusion cycles equals ω^{-1}. The current experimental and theoretical uncertainty, at least for the dt fusion process, brackets the difference between possibility or impossibility of building and operating muon-catalyzed fusion reactors efficiently.

A precise prediction of ω requires an accurate knowledge of the three-body mesomolecular wave function. The usually employed adiabatic approaches,[4,5] which assume an instant muonic response to nuclear motion, are not extremely precise, since the mass of the muon is not very small compared to the masses of nucleons. Variational wave functions,[6,7] on the other hand, 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 calculations[8] for ground states do not have these limitations, but their 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 importance function will eventually dominate the numerical simulation. In view of the difficulties of the above-mentioned approaches, we propose applying the correlation-function hyperspherical harmonic (CFHH) method,[9-12] which, in principle, can generate accurate ground- and excited-state wave functions for all interparticle distances, including coalescence points, to mesomolecular systems.

To date, the accuracy of this method has been verified for systems consisting of one heavy and two light particles, and of particles of equal masses. Direct solution of the Schrödinger equation by the CFHH method for bound three-body atomic systems has yielded precision[9-12] comparable to that obtained previously only by elaborate variational calculations. For maximum global momentum $K_m=48$, up to nine-significant-figure precision has been obtained for the energy of the helium atom[9-11] and seven significant figures for the positronium ion[12] $e^-e^-e^+$ (also denoted Ps^-). The wave functions for the whole range of the interparticle distances and different expectation values for these systems have about six- and five-significant-figure precision, respectively.

In this paper we extend our study of the CFHH method to the ground S states of the $pp\mu$, $dd\mu$, and $tt\mu$ molecular ions. This is our first test of the method for heavy-heavy-light systems. This is also a prelude to investigating P states of the $dd\mu$ and $dt\mu$ molecular ions whose properties are of most relevance for muon-catalyzed fusion research.

In the CFHH method[9-12] we write the wave function as a production of two factors

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

where χ is the "correlation function" and ϕ is expanded in the usual hyperspherical harmonic (HH) functions. If the correlation function χ is chosen to describe the singular features of ψ (like cusps), the HH expansion for ϕ should be rapid. The solution for ϕ proceeds as in the usual HH method, except 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 $xx\mu$ systems ($x=p,d,t$) we employ correlation functions $\chi=\exp(f)$ of the simple spatially symmetric form

$$f=-\gamma(r_{13}+r_{23})-\delta r_{12} \ , \tag{3}$$

TABLE I. Calculated ground-state binding energy ε, its expectation value $\langle h \rangle$, and different functions of interparticle distances, in eV and absolute muonic atomic units $a_\mu = 2.559\,277\ 10^{-13}$ m, respectively. The index 3 indicates a 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 correlation parameters $\gamma = 0$ and $\delta = 0$ correspond to the standard hyperspherical harmonic method.

K_m	N	$\langle r_{12}^{-2} \rangle$	$\langle r_{12}^{-1} \rangle$	$10^6 \langle \delta(\mathbf{r}_{12}) \rangle$	$\langle r_{12} \rangle$	$\langle r_{12}^2 \rangle$	ε
12	16	0.26	0.48	538.0	2.33	5.96	−119[a]
16	25	0.24	0.46	46.9	2.40	6.32	21.5
20	36	0.23	0.45	10.0	2.47	6.65	112.5
K_m	N	$\langle r_{13}^{-2} \rangle$	$\langle r_{13}^{-1} \rangle$	$\langle \delta(\mathbf{r}_{13}) \rangle$	$\langle r_{13} \rangle$	$\langle r_{13}^2 \rangle$	
12	16	0.81	0.69	0.052	1.98	4.94	
16	25	0.87	0.71	0.061	1.97	4.90	
20	36	0.92	0.72	0.070	1.97	4.99	

[a]Unbound.

where particle 3 is the unlike mass.

Tables I–III show the results for different choices of γ and δ for the $dd\mu$ molecular ion. The binding energies are given in eV and expectation values in muonic atomic units[13] $a_\mu = 2.559\,277\ 10^{-13}$ m. Tables IV and V give the results for the $pp\mu$ and $tt\mu$ molecular ions. Also included are the results of calculations for the binding energies[15–22,24] and available expectation values[13,14] obtained by other methods. In our calculations the following values of proton, deuteron, tritium, and muon masses and of the Rydberg constant $\mathcal{R}$ were used:

$$m_\mu = 206.769 m_e, \quad m_p = 1836.1515 m_e ,$$
$$m_d = 3670.481 m_e, \quad m_t = 5496.918 m_e , \tag{4}$$
$$\mathcal{R} = 13.605\,804\,1 \text{ eV} .$$

This set of values is one of the most commonly used in muonic molecule binding energy calculations.

The choice $\gamma = \delta = 0$ in Table I corresponds to the usual HH method. Another choice, displayed in Table II, is the "uncorrelated variational" choice[25] $\delta = 0$, $\gamma = 11M/[16(M+1)]$. This value of γ corresponds[15] to the correlation function χ giving the minimum energy with the restriction $\delta = 0$. A third choice of parameters γ and δ is employed in Tables III–V. Here the parameter $\gamma = M/(M+1)$ builds in the μd cusps[26] and δ is chosen to be such that for $K_m = 0$, the full wave function ψ asymptotically has the correct cluster structure. This means (i) ψ decays exponentially for any r_{ij} going to infinity; and (ii) for r_{13} (or r_{23}) going to infinity ψ decays at a rate appropriate for particle 1 (or 2) bound loosely to the ground state of the particles 2 and 3 (or 1 and 3), i.e.,

$$\psi \sim \exp\{-[(2M+2)(|E_{xx\mu}| - |E_{x\mu}|)/(m+2)]^{1/2} r_{13}\} ,$$

where $E_{x\mu}$ and $E_{xx\mu}$ are the two and three particle energies, respectively. Of course, the exact value of δ then depends on $E_{xx\mu}$, which is what we are trying to calculate. We do know however, that $|E_{xx\mu}| > |E_{x\mu}|$, and also that the parameter δ has to be chosen only approximately equal to its correct value. The choices of δ we actually

TABLE II. Same as in Table I. The correlation parameters in absolute muonic atomic units a_μ^{-1} are $\gamma = 0.6508$ and $\delta = 0$ (uncorrelated variational parametrization).

K_m	N	$\langle r_{12}^{-2} \rangle$	$\langle r_{12}^{-1} \rangle$	$10^6 \langle \delta(\mathbf{r}_{12}) \rangle$	$\langle r_{12} \rangle$	$\langle r_{12}^2 \rangle$	ε
12	16	0.20	0.408	4.81	2.64	7.93	194.34
16	25	0.20	0.420	4.72	2.65	7.71	205.76
20	36	0.20	0.417	4.27	2.67	7.83	235.43
24	49	0.19	0.414	3.91	2.69	7.95	259.28
28	64	0.19	0.411	3.67	2.71	8.05	274.23
K_m	N	$\langle r_{13}^{-2} \rangle$	$\langle r_{13}^{-1} \rangle$	$\langle \delta(\mathbf{r}_{13}) \rangle$	$\langle r_{13} \rangle$	$\langle r_{13}^2 \rangle$	$\langle h \rangle$
12	16	0.98	0.710	0.106	2.03	5.36	273.2
16	25	1.03	0.722	0.116	2.03	5.36	290.21
20	36	1.06	0.726	0.122	2.05	5.44	303.10
24	49	1.08	0.729	0.127	2.05	5.50	309.48
28	64	1.09	0.730	0.130	2.06	5.54	313.14

TABLE III. Same as in Table I. The correlation parameters are $\gamma=0.9467$ and $\delta=4.172$ (μd cusp parametrization). The last lines of the table contain the results of precision calculations obtained by other methods.

K_m	N	$\langle r_{12}^{-2}\rangle$	$\langle r_{12}^{-1}\rangle$	$10^6\langle\delta(\mathbf{r}_{12})\rangle$	$\langle r_{12}\rangle$	$\langle r_{12}^2\rangle$	ε
12	16	0.21	0.436	19	2.5	7.0	309.793 98
16	25	0.168	0.3843	3.8	2.92	9.47	355.893 54
20	36	0.173	0.3895	3.30	2.88	9.17	341.387 80
24	49	0.175	0.3918	3.25	2.86	9.03	334.410 52
28	64	0.176 32	0.393 197	3.212	2.8465	8.9554	329.800 16
32	81	0.176 815	0.393 754	3.147 83	2.842 38	8.9291	327.623 14
40	121	0.177 209	0.394 211	3.011 70	2.838 82	8.9058	326.333 80
48	169	0.177 458	0.394 502	2.919 40	2.836 45	8.8900	325.605 94

Reference	$\langle r_{12}^{-1}\rangle$	$\langle r_{12}\rangle$	$\langle r_{12}^2\rangle$
13		2.834	8.876
14	0.394	2.834	8.877

K_m	N	$\langle r_{13}^{-2}\rangle$	$\langle r_{13}^{-1}\rangle$	$\langle\delta(\mathbf{r}_{13})\rangle$	$\langle r_{13}\rangle$	$\langle r_{13}^2\rangle$	$\langle h\rangle$
12	16	1.24	0.7725	0.175	2.0	5.1	297.8
16	25	1.11	0.7210	0.157	2.15	6.12	319.8
20	36	1.148	0.7273	0.1599	2.14	6.08	323.9
24	49	1.146	0.7278	0.1594	2.13	6.01	324.66
28	64	1.145 913	0.728 079	0.159 103 6	2.1246	5.9774	324.8450
32	81	1.145 460	0.728 157	0.158 961 3	2.123 18	5.968 11	324.966 65
40	121	1.145 744	0.728 312	0.158 952 7	2.121 82	5.958 98	325.029 41
48	169	1.145 502	0.728 400	0.158 839 4	2.120 82	5.952 23	325.054 88

Reference	$\langle r_{13}^{-1}\rangle$	$\langle r_{13}\rangle$	$\langle r_{13}^2\rangle$	$\langle h\rangle$
13,15		2.12	5.945	325.0735
14,16	0.7285	2.12	5.946	325.0735
17				319.2
18				322
19				318
20				306

TABLE IV. Same as in Table III, but for $pp\mu$ molecular ion. The correlation parameters are $\gamma=0.8988$ and $\delta=2.220$.

K_m	N	$\langle r_{12}^{-2}\rangle$	$\langle r_{12}^{-1}\rangle$	$10^5\langle\delta(\mathbf{r}_{12})\rangle$	$\langle r_{12}\rangle$	$\langle r_{12}^2\rangle$	ε
12	16	0.149	0.353	5.9	3.26	12.0	272.062 60
16	25	0.145	0.346	5.36	3.37	13.1	264.541 98
20	36	0.147 70	0.3506	5.26	3.312	12.5	257.379 31
24	49	0.148 017	0.350 926	5.080	3.3095	12.47	255.289 74
28	64	0.148 241	0.351 212 9	4.930 396	3.306 37	12.447	254.579 03
32	81	0.148 432 85	0.351 457 59	4.817 149	3.303 684	12.425	253.966 92
40	121	0.148 593 12	0.351 662 37	4.652 784	3.301 436	12.406 719	253.476 63
48	169	0.148 661 87	0.351 751 70	4.542 995	3.300 421	12.398 301	253.294 76

Reference	$\langle r_{12}^{-1}\rangle$	$\langle r_{12}\rangle$	$\langle r_{12}^2\rangle$
13		3.298	12.38
14	0.351	3.299	12.39

K_m	N	$\langle r_{13}^{-2}\rangle$	$\langle r_{13}^{-1}\rangle$	$\langle\delta(\mathbf{r}_{13})\rangle$	$\langle r_{13}\rangle$	$\langle r_{13}^2\rangle$	$\langle h\rangle$
12	16	0.9882	0.672	0.1318	2.35	7.4	229
16	25	0.9868	0.668	0.1321	2.42	8.1	252.6
20	36	0.996 59	0.6700	0.131 78	2.390	7.80	252.940
24	49	0.996 110	0.669 999	0.131 685	2.3901	7.8061	253.0712
28	64	0.996 167 88	0.670 111 0	0.131 687 45	2.388 73	7.7950	253.104 18
32	81	0.995 980 67	0.670 179 97	0.131 612 39	2.387 534	7.785 05	253.124 68
40	121	0.996 007 50	0.670 242 71	0.131 568 24	2.386 562 16	7.777 020 7	253.143 08
48	169	0.995 935 46	0.670 272 62	0.131 535 70	2.386 098 56	7.773 144 9	253.148 24

TABLE IV. (*Continued*).

Reference	$\langle r_{13}^{-1} \rangle$	$\langle r_{13} \rangle$	$\langle r_{13}^{2} \rangle$	$\langle h \rangle$
13		2.385	7.769	253.1523
14	0.6703	2.386	7.769	253.1524
17				252.9
18				242
19				249
20				230

employ are appropriate for $|E_{xx\mu}|$ about 5% higher than $|E_{x\mu}|$.

As one can see from the Tables I–III this "μd cusp" parametrization gives the best results for binding energies $\varepsilon = -(E - E_{x\mu})$, the expectation value of binding energy $\langle h \rangle$, $h = -(H - E_{x\mu})$, and for all other expectation values. (As described in our previous work,[9] E, the eigenvalue of the effective Schrödinger equation, differs from $\langle H \rangle$, the expectation 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 results in Table III clearly illustrate the utility of the CFHH method in $dd\mu$ computations. Indeed, values presented here are better than those obtained by adiabatic method[17] or in variational calculations[18–20] with the Hylleraas-type variational wave functions. They agree with the most sophisticated variational calculations using the Slater-type geminals[13,15,22,24] and the generator-

TABLE V. Same as in Table III, but for $tt\mu$ molecular ion. The correlation parameters are $\gamma = 0.9637$ and $\delta = 6.115$.

K_m	N	$\langle r_{12}^{-2} \rangle$	$\langle r_{12}^{-1} \rangle$	$10^6 \langle \delta(\mathbf{r}_{12}) \rangle$	$\langle r_{12} \rangle$	$\langle r_{12}^{2} \rangle$	ε
12	16	0.337	0.556		1.91	3.86	251.535 95
16	25	0.182	0.402		2.78	8.62	409.413 36
20	36	0.185 23	0.407 75	45.0	2.696	7.91	390.783 00
24	49	0.186 69	0.409 33	2.7	2.687	7.87	380.269 44
28	64	0.188 22	0.411 11	0.41	2.674	7.78	374.062 90
32	81	0.189 22	0.412 01	0.387	2.6669	7.745	369.597 71
40	121	0.190 28	0.413 36	0.424	2.659 23	7.7006	365.209 84
48	169	0.190 68	0.413 82	0.307	2.655 72	7.6780	364.143 20

Reference	$\langle r_{12}^{-1} \rangle$	$10^6 \langle \delta(\mathbf{r}_{12}) \rangle$	$\langle r_{12} \rangle$	$\langle r_{12}^{2} \rangle$
13			2.652 82	7.662 14
14	0.414	0.297 93	2.653	7.662

K_m	N	$\langle r_{13}^{-2} \rangle$	$\langle r_{13}^{-1} \rangle$	$\langle \delta(\mathbf{r}_{13}) \rangle$	$\langle r_{13} \rangle$	$\langle r_{13}^{2} \rangle$	$\langle h \rangle$
12	16	1.536	0.890	0.222	1.59	3.26	129.0
16	25	1.159	0.744	0.169	2.06	5.59	367.98
20	36	1.210	0.7518	0.1711	2.031	5.39	361.06
24	49	1.212	0.7524	0.1716	2.0301	5.40	361.90
28	64	1.2116	0.752 88	0.171 33	2.0251	5.360	362.257
32	81	1.210 43	0.753 007	0.170 931	2.022 66	5.3455	362.566
40	121	1.209 79	0.753 195	0.170 589	2.019 97	5.3288	362.812
48	169	1.209 96	0.753 395	0.170 601	2.018 52	5.3192	362.856

Reference	$\langle r_{13}^{-1} \rangle$	$\langle r_{13} \rangle$	$\langle r_{13}^{2} \rangle$	$\langle h \rangle$
13,15,21		2.017 37	5.312 90	362.910 304
14,16	0.7535	2.017	5.313	362.909 45
22				362.904
23				362.910 29

coordinate method,[14,16] with the precision of our calculations converged, for example, for the expectation values of binding energy up to an error in the fifth significant figure. The results of $pp\mu$ and $tt\mu$ calculations, obtained with the same kind of parametrization and displayed in Tables IV and V, confirm the utility of the method.

Improvements in the CFHH method are nevertheless desirable for the $dd\mu$ and other heavy-heavy-light particle systems. It is impossible to build in both a satisfactory asymptotic behavior and xx cusp behavior with the symmetric linear correlation factor f we have chosen. This situation becomes worse with increasing mass of the particle x. The reason is that the x-x cusp parameters $\delta=-0.5$ in the units $m_x=1$ becomes -4.442, -8.878, and -13.298 in μ atomic units for $x=p$, d and t, respectively, whereas the δ, actually used, given in Tables III–V and chosen, as discussed earlier, on the basis of asymptotic considerations, become increasingly positive with m_x. Correspondingly, the discrepancy in binding energies with the very accurate variational calculations[15,16] are 4, 19, and 60 meV, respectively, and convergence of $\langle \delta(\mathbf{r}_{12}) \rangle$ becomes progressively worse. Also, an additional numerical difficulty[11] in extracting the asymptotic wave function leads to not being able to obtain precision in expectation values better than the number of significant figures shown in the table for the uncorrelated variational or μd cusp parametrizations of f.

As previously mentioned, the inability with current correlation factors to include the xx cusp leads to somewhat slow convergence of $\langle \delta(r_{12}) \rangle$. However, a matrix element of the $\delta(\mathbf{r}_{12})$ operator is directly connected[27] with the muon-sticking probability in the sudden approximation. For this reason we plan to consider more general nonsymmetric nonlinear correlation functions for $pp\mu$, $dd\mu$, $tt\mu$, and $dt\mu$ molecular ions, which will properly describe both xx and dt cusps and asymptotic behavior.[26] That will allow a very precise estimate of wave functions at xx and dt coalescence points, which is necessary for an accurate calculation of the sticking probabilities.

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