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Geometries of muonic molecular ions

A. Scrinzi, H. J. Monkhorst, and S. A. Alexander
Quantum Theory Project, Department of Physics and Department of Chemistry, University of Florida, Gainesville, Florida 32611
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For the $J=0,1$ bound states of the muonic ions $xy\mu$ $(x,y=p,d,t)$ we calculate the expectation values of the interparticle distances and of the distances squared. We find that the $J=1$ excited states of $td\mu$ and $dd\mu$ are quite large in comparison to all the other states.

I. INTRODUCTION

A number of large variational calculations have recently obtained highly accurate binding energies for the $J=0,1$ bound states of the muonic molecular ions $td\mu$ and $dd\mu$ (see, for example, Refs. 1–8). These systems are of particular interest because of their importance to the process of muon-catalyzed fusion. In addition to the binding energies, each variational calculation can also produce a wave function with which one can study properties of more physical interest, e.g., the probability of the muon sticking to the alpha particle after fusion (see, for example, Refs. 9–12). In this paper we examine another property of interest, the arrangement of the three bodies within each ion. This information provides a firm basis for understanding the formation and the physical interaction of the ion with its electronic surroundings. In particular, the first excited $J=1$ states of $td\mu$ and $dd\mu$ are expected to be of non-negligible size when compared to the electronic molecules (see Ref. 13). For this reason we have calculated the expectation values of the interparticle distances and of the distances squared of these two states. To put these numbers in a clearer perspective we have also calculated these quantities for the other muonic ions. For simplicity, we shall hereafter refer to each bound state simply as $xy\mu(m,n)$, where the label m denotes the angular-momentum ($0=S$, $1=P$) and n specifies whether the state is the ground state ($n=0$) or the first excited state ($n=1$).

II. CALCULATIONS AND RESULTS

For the wave functions of each ion we use the various sets of explicitly correlated Slater-type geminals computed in Ref. 1 with mass set 2 ($m_t=5496.918m_e$, $m_d=3670.481m_e$, $m_\mu=206.7686m_e$). These have the form

$$\Psi=(1+P_{12})\sum_{i=1}^{K}c_i\exp(-\alpha_i r_{x\mu}-\beta_i r_{y\mu}-\gamma_i r_{xy}) \quad (1)$$

for homonuclear S states,

$$\Psi=\sum_{i=1}^{K}c_i\exp(-\alpha_i r_{x\mu}-\beta_i r_{y\mu}-\gamma_i r_{xy}) \quad (2)$$

for heteronuclear S states,

$$\Psi=(1-P_{12})\sum_{i=1}^{K}c_i r_{x\mu}\cos\theta_1\exp(-\alpha_i r_{x\mu}-\beta_i r_{y\mu}-\gamma_i r_{xy}) \quad (3)$$

for homonuclear P states,

$$\Psi=\sum_{i=1}^{K/2}c_i r_{x\mu}\cos\theta_1\exp(-\alpha_i r_{x\mu}-\beta_i r_{y\mu}-\gamma_i r_{xy})+\sum_{j=1}^{K/2}\hat{c}_j r_{y\mu}\cos\theta_2\exp(-\alpha_j r_{x\mu}-\beta_j r_{y\mu}-\gamma_j r_{xy}) \quad (4)$$

for heteronuclear P states, where $r_{x\mu}$ and $r_{y\mu}$ are the distances between the muon to particle x and y, respectively, r_{xy} is the distance between x and y, and P_{12} is the operator that interchanges $r_{x\mu}$ and $r_{y\mu}$. The nonlinear parameters (α_i, β_i, and γ_i) are chosen using random tempering formulas. This method enabled us to systematically increase the size of the basis set until the binding energies of all states converged to about 1 μeV except for the $td\mu(1,1)$ state. This state converged much slower than the others and was only accurate to about 10^{-4} eV.

In Table I we show that the convergence of the expectation values of the interparticle distances is roughly the same as those for the binding energies. This is true not only for the best converged state, $tt\mu(0,0)$, but also the worst converged state, $td\mu(1,1)$. The distances in this table are given in "natural muonic" units, i.e., $\hbar=e=\mu_x=1$ where $\mu_x=m_\mu M_x(m_\mu+M_x)$ is the reduced mass of the muon-x system and where x is the

TABLE I. Comparison of the convergence of the binding energy (BE) and of the interparticle distances for the $tt\mu(0,0)$ and $td\mu(1,1)$ states. K is the number of basis functions used. The distances are in natural muonic units and the binding energies are in eV.

	K	BE	$\langle r_{x\mu}\rangle$	$\langle r_{y\mu}\rangle$	$\langle r_{xy}\rangle$
$tt\mu(0,0)$	100	362.907 297 7	1.944 257 437 23	1.944 257 437 23	2.556 687 765 86
	200	362.909 758 1	1.944 240 582 80	1.944 240 582 80	2.556 656 286 59
	300	362.909 768 8	1.944 240 496 01	1.944 240 496 01	2.556 656 102 27
	400	362.909 769 6	1.944 240 489 33	1.944 240 489 33	2.556 656 088 57
	500	362.909 769 6	1.944 240 488 80	1.944 240 488 80	2.556 656 087 55
$td\mu(1,1)$	1200	0.659 976 8	2.225 318 762 66	8.348 893 568 41	9.068 975 727 61
	1400	0.660 090 5	2.225 152 989 33	8.358 521 874 75	9.078 435 186 10
	1800	0.660 161 7	2.225 061 524 72	8.364 804 312 25	9.084 635 353 34
	2000	0.660 172 1	2.224 967 159 71	8.366 607 099 46	9.086 374 206 51

most massive particle. Because the wave functions have been computed in these units, this choice has a certain simplistic appeal. Unfortunately the dependence of these units on M_x makes it difficult to directly compare the expectation values of different ions since the most massive particle may not be tritium. One alternative is to use "absolute muonic" units where $m_\mu = 1$. This set of units is independent of the particles selected and will be used in the rest of our calculations. In Table II we give the expectation values of the distances and the distances squared for all the muonic ions considered in Ref. 1. The expectation values of the distances squared are of particular use in calculations of corrections of the interaction of the muonic molecular ion with the surrounding electrons [compare Eqs. (1.8) and 2.8) in Ref. 13]. For completeness we also give the computed binding energies of each system. The expectation values of the distances show that the $td\mu(1,1)$ and $dd\mu(1,1)$ states are physically quite large in comparison to all the other states. They also show that the $td\mu(1,1)$ state has very much the character of a $t\mu+d$ system. Since his basis set explicitly included terms of this type, this may explain why the coupled-channel calculations of Kamimura[5] converged relatively rapidly and had little problem with linear dependence.

Also included in Table II is a calculation of

$$\delta_{xy} = \Delta_{xy} / \langle r_{xy} \rangle \ , \tag{5}$$

where

$$\begin{aligned} \Delta xy &= (\langle r_{xy}^2 \rangle - \langle r_{xy} \rangle^2)^{1/2} \\ &= \langle (r_{xy} - \langle r_{xy} \rangle)^2 \rangle^{1/2} \ . \end{aligned} \tag{6}$$

TABLE II. Expectation values of the interparticle distances and the distances squared of the muonic molecular ions $xy\mu$ $(x,y = p,d,t)$. The accuracy is estimated to be ± 2 in the last digit or better. The distances are in absolute muonic units, i.e,. $a_\mu = m_e/m_\mu a_0 = 255.927\,70 \times 10^{-15}$ m. Binding energies (BE) are in eV. $\delta_{xy} = \Delta_{xy}/\langle r_{xy}\rangle$, where $\Delta_{xy} = (\langle r_{xy}^2\rangle - \langle r_{xy}\rangle^2)^{1/2}$.

	BE	$\langle r_{x\mu}\rangle$	$\langle r_{y\mu}\rangle$	$\langle r_{xy}\rangle$	$\langle r_{x\mu}^2\rangle$	$\langle r_{y\mu}^2\rangle$	$\langle r_{xy}^2\rangle$	δ_{xy}
$tt\mu(0,0)$	362.9097	2.017 37	20.17 37	2.652 82	5.312 90	5.312 90	7.662 14	0.297 93
$tt\mu(0,1)$	83.7712	2.965 84	2.965 84	4.453 66	12.8861	12.8861	22.4769	0.364 95
$tt\mu(1,0)$	289.1417	2.1231	2.1231	2.8648	5.9059	5.9059	8.9042	0.291 44
$tt\mu(1,1)$	45.2058	3.242	3.242	5.003	15.81	15.81	28.41	0.367 47
$td\mu(0,0)$	319.1397	2.0237	2.1178	2.7479	5.3970	5.8818	8.2872	0.312 25
$td\mu(0,1)$	34.8344	2.738	3.933	5.161	11.75	22.39	30.61	0.386 20
$td\mu(1,0)$	232.4715	2.1567	2.2806	3.0272	6.1890	6.8751	10.0185	0.305 37
$td\mu(1,1)$	0.6601	2.308	8.67	9.428	9.243	128.9	133.0	0.704 47
$dd\mu(0,0)$	325.0735	2.120	2.120	2.834	5.945	5.945	8.876	0.324 25
$dd\mu(0,1)$	35.8443	3.616 30	3.616 30	5.694 74	20.5410	20.5410	37.4188	0.392 21
$dd\mu(1,0)$	226.6816	2.2862	2.2862	3.1668	6.9693	6.9693	11.031	0.316 15
$dd\mu(1,1)$	1.9748	5.416	5.416	9.270	58.5	58.5	112.0	0.550 76
$tp\mu(0,0)$	213.8401	2.002 01	2.461 28	3.036 54	5.4044	8.031	10.347	0.349 52
$tp\mu(1,0)$	99.1265	2.1381	2.9027	3.5846	6.3136	11.3517	14.4619	0.354 25
$dp\mu(0,0)$	221.5494	2.0876	2.4514	3.1007	5.8965	8.0334	10.8291	0.355 25
$dp\mu(1,0)$	97.4981	2.264 80	2.919 93	3.712 64	7.135 61	11.6455	15.5614	0.359 12
$pp\mu(0,0)$	253.1523	2.385	2.385	3.298	7.769	7.769	12.38	0.371 75
$pp\mu(1,0)$	107.2659	2.7790	2.7790	4.0822	10.8982	10.8982	18.9828	0.372 99

TABLE III. Expectation values of the muonic molecular ions $xy\mu$ using other wave functions. The distances are in absolute muonic units, i.e., $a_\mu = m_e/m_\mu a_0 = 255.927\,70 \times 10^{-15}$ m.

	$\langle r_{x\mu} \rangle$	$\langle r_{y\mu} \rangle$	$\langle r_{xy} \rangle$	$\langle r_{x\mu}^2 \rangle$	$\langle r_{y\mu}^2 \rangle$	$\langle r_{xy}^2 \rangle$
			Wave functions from Refs. 2 and 9			
$td\mu(0,0)$	2.023	2.117	2.747			
$td\mu(0,1)$	2.738	3.933	5.161			
$td\mu(1,0)$	2.157	2.280	3.027			
$td\mu(1,1)$	2.308	8.678	9.42			
			Results from Ref. 14			
$tt\mu(0,0)$	2.017	2.017	2.653	5.313	5.313	7.662
$tt\mu(0,1)$	2.966	2.966	4.454	12.89	12.89	22.48
$td\mu(0,0)$	2.024	2.118	2.748	5.396	5.882	8.287
$td\mu(0,1)$	2.737	3.915	5.142	11.74	22.12	30.34
$dd\mu(0,0)$	2.120	2.120	2.834	5.946	5.946	8.877
$dd\mu(0,1)$	3.616	3.616	5.695	20.54	20.54	27.42
$tp\mu(0,0)$	2.002	2.461	3.036	5.405	8.031	10.35
$dp\mu(0,0)$	2.088	2.451	3.101	5.896	8.033	10.83
$pp\mu(0,0)$	2.886	2.886	3.299	7.769	7.769	12.39

Δ_{xy} is the root-mean-square deviation of the x-y distance from the equilibrium value $\langle r_{xy} \rangle$. Since we consider several systems, we scale this quantity by $\langle r_{xy} \rangle$ to place them all on an equal footing. Except for the very loosely bound states, we find that all of the values of δ_{xy} lie between 0.29 and 0.39. This suggests that the muonic ions are far from being rigid structures and that any attempt to describe them as such should be done cautiously. This is especially true of the very diffuse $dd\mu(1,1)$ and $td\mu(1,1)$ states which have values of $\delta_{xy} = 0.55$ and 0.70, respectively.

We have also noticed that the computational effort associated with the muonic ions increases with the size of δ_{xy}. Although the rates are different for the $J=0$ and 1 systems, those states that converged slowly in Ref. 1 have, without exception, the largest values of δ_{xy}. We believe that this is because these states also have large values of $\langle r_{xy} \rangle$ and that in order to accurately describe such diffuse systems one needs a wide range of γ in a basis of Slater-type geminals (which are monotonically decreasing functions) and thus a large expansion.

As a check of our results, we first examined the effect of small changes in the particle masses. Since Ref. 1 computed the binding energies of $td\mu$ with the two most widely used tritium masses, $m_t = 5496.918 m_e$ and $5496.899 m_e$, we took both sets of wave functions and calculated a number of expectation values. We found no difference between these calculations to within the estimated convergence. Next we calculated the distances of the $td\mu$ molecular ion using the wave functions from a very accurate series of calculations by Szalewicz and coworkers.[2,9] This work used a generalized Hylleraas basis set. Although quite different from the basis set used in Ref. 1, the results are in good agreement with those in Table II.

In addition to the work presented here the expectation values of the distances and of the distances squared have recently been computed by Petelenz and Smith[14] for all of the $J=0$ states. For comparison, we present their results in Table III. Although their wave function is formally identical to Eqs. (1) and (2) above, they used a different tempering method to select their nonlinear parameters. With the exception of some of the $td\mu(0,1)$ calculations, these results are in full agreement with ours to within the estimated convergence of our results. We believe that the differences are due entirely to the quality of the wave functions for this state. As we showed above, the convergence of the binding energy is strongly related to the convergence of the expectation values. In Ref. 7 Petelenz and Smith give a value of 34.823 81 eV for the binding energy of the $td\mu(0,1)$ state. Since this amount has only converged to about three significant figures, one should not expect the expectation values to be accurate to more than two or three significant figures.

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