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Variational calculation of the energy levels of the $(dt\mu)^+$ molecule

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The ground and the excited states of both the s and p states of the $(dt\mu)^+$ molecule are calculated using the variational method of moments. Our best energy values are -319.117 and -34.776 eV for the s states, and -232.436 and -0.628 eV for the p states.

I. INTRODUCTION

Nonvariational calculations of mesic molecular spectra have been reported by Vinitiskii *et al.*¹ More recently, a three-body variational calculation for these spectra using Hylleraas wave functions has been carried out by Bhatia and Drachman.² The latter calculation generally agrees with that of Ref. 1 except that for the excited p state of the $(dt\mu)^+$ molecule, Bhatia and Drachman obtained -0.224 eV in a 440-term expansion while a value of -0.64 eV was reported in Ref. 1. This large discrepancy led people to doubt the usefulness of the variational method to calculate such weakly bound states.

We have carried out a calculation of all the energy levels of the $(dt\mu)^+$ molecule, using our variational method of moments.³ Our calculation indicates that with a properly chosen set of basis functions, considerably faster convergence can be achieved. Our present set of basis functions converges twice as fast as the Hylleraas expansion in Ref. 2. For example, our 390-term expansion gives -0.437 eV for the excited p state in comparison with their 440-term value of -0.224 eV. For better excited- p -state energy, proper

rearrangement of the trial functions is necessary. We have increased the number of terms that correspond to configurations where the two nuclei are in relative p states and reduced the number of terms that correspond to configurations where the two nuclei are in relative s states. In doing so we are able to obtain -0.628 eV, thus reducing the discrepancy between the variational result and that of Ref. 1 to less than 2% and to less than 4% when compared with the most recent value of -0.656 eV.⁴

As in Ref. 3, our variational calculation requires two iterations. Convergent results are obtained when there are six or more digits in common amongst the variational energies from the first moment, the second moment, and the variational bounds obtained from the method of moments.

II. THREE-BODY PROBLEM WITH UNEQUAL MASSES

A. s state

Our s -state variational wave function is

$$\Psi_s = \sum_{n_1 n_2 n_3} C_{(n_1 n_2 n_3)} r_{12}^{n_1} r_{13}^{n_2} r_{23}^{n_3} \{ \exp[-(a_1 r_{12} + a_2 r_{13} + a_3 r_{23})] + \exp[-(b_1 r_{12} + b_2 r_{13} + b_3 r_{23})] \} . \quad (1)$$

The corresponding kinetic energy operator, the kinetic energy divided by $-\hbar^2$, is

$$K_0 = \frac{1}{2\mu_{12}} \left(\frac{2}{r_{12}} \frac{\delta}{\delta r_{12}} + \frac{\delta^2}{\delta r_{12}^2} \right) + \frac{1}{m_1} \frac{r_{13}^2 + r_{12}^2 - r_{23}^2}{2r_{12}r_{13}} \frac{\delta^2}{\delta r_{12}\delta r_{13}} + \frac{1}{2\mu_{23}} \left(\frac{2}{r_{23}} \frac{\delta}{\delta r_{23}} + \frac{\delta^2}{\delta r_{23}^2} \right) \\ + \frac{1}{m_2} \frac{r_{12}^2 + r_{23}^2 - r_{13}^2}{2r_{12}r_{23}} \frac{\delta^2}{\delta r_{12}\delta r_{23}} + \frac{1}{2\mu_{13}} \left(\frac{2}{r_{13}} \frac{\delta}{\delta r_{13}} + \frac{\delta^2}{\delta r_{13}^2} \right) + \frac{1}{m_3} \frac{r_{13}^2 + r_{23}^2 - r_{12}^2}{2r_{13}r_{23}} \frac{\delta^2}{\delta r_{13}\delta r_{23}} , \quad (2)$$

where μ_{ij} are the reduced masses between particles i and j . r_{ij} are the interparticle distances.

B. p state

Our p -state wave function is $\Psi_p = f_1 \mathbf{p} + f_2 \mathbf{r}$, where \mathbf{p} and \mathbf{r} are the Jacobian coordinates for unequal masses. Particle 1 is triton, particle 2 is deuteron, particle 3 is the muon, and

$$\begin{aligned}
 f_1 &= \sum_{n_1, n_2, n_3} C_{(n_1, n_2, n_3)} r_{12}^{n_1} r_{13}^{n_2} r_{23}^{n_3} \{ \exp[-(a_1 r_{12} + a_2 r_{13} + a_3 r_{23})] + \exp[-(b_1 r_{12} + b_2 r_{13} + b_3 r_{23})] \}, \\
 f_2 &= \sum_{n_1, n_2, n_3} d_{(n_1, n_2, n_3)} r_{12}^{n_1} r_{13}^{n_2} r_{23}^{n_3} \{ \exp[-(a_1 r_{12} + a_2 r_{13} + a_3 r_{23})] - \exp[-(b_1 r_{12} + b_2 r_{13} + b_3 r_{23})] \}.
 \end{aligned}
 \tag{3}$$

The corresponding modified kinetic energy operator which operates directly on f_1 and f_2 is

$$K = \begin{pmatrix} K_{11} & K_{12} \\ K_{21} & K_{22} \end{pmatrix},$$

after integration over orientations, where

$$\begin{aligned}
 K_{11} &= r_{12}^2 K_0 + \frac{1}{\mu_{12}} r_{12} \frac{\delta}{\delta r_{12}} + \frac{1}{2m_1} \frac{r_{12}^2 + r_{13}^2 - r_{23}^2}{r_{13}} \frac{\delta}{\delta r_{13}} + \frac{1}{2m_1} \frac{r_{12}^2 + r_{23}^2 - r_{13}^2}{r_{23}} \frac{\delta}{\delta r_{23}}, \\
 K_{12} &= \left[\left(\frac{m_1}{Mm_2m_3} \right)^{1/2} \frac{r_{12}^2 + r_{13}^2 - r_{23}^2}{4} - \left(\frac{m_2}{Mm_1m_3} \right)^{1/2} \frac{r_{12}^2 + r_{23}^2 - r_{13}^2}{4} \right] K_0 \\
 &\quad + \left(\frac{M}{m_1m_2m_3} \right)^{1/2} \left[\frac{r_{12}^2 + r_{13}^2 - r_{23}^2}{2r_{13}} \frac{\delta}{\delta r_{13}} - \frac{r_{12}^2 + r_{23}^2 - r_{13}^2}{2r_{23}} \frac{\delta}{\delta r_{23}} \right], \\
 K_{21} &= \left[\left(\frac{m_1}{Mm_2m_3} \right)^{1/2} \frac{r_{12}^2 + r_{13}^2 - r_{23}^2}{4} - \left(\frac{m_2}{Mm_1m_3} \right)^{1/2} \frac{r_{12}^2 + r_{23}^2 - r_{13}^2}{4} \right] K_0 \\
 &\quad + \frac{1}{2\mu_{12}} \left[\left(\frac{m_1m_2}{Mm_2} \right)^{1/2} (r_{12}^2 + r_{13}^2 - r_{23}^2) - \left(\frac{m_2m_3}{Mm_1} \right)^{1/2} (r_{12}^2 + r_{23}^2 - r_{13}^2) \right] \frac{1}{r_{12}} \frac{\delta}{\delta r_{12}} \\
 &\quad + \frac{1}{2m_1} \left[2 \left(\frac{m_1m_3}{Mm_2} \right)^{1/2} r_{13}^2 + \left(\frac{m_2m_3}{Mm_1} \right)^{1/2} (r_{13}^2 + r_{23}^2 - r_{12}^2) \right] \frac{1}{r_{13}} \frac{\delta}{\delta r_{13}} \\
 &\quad - \frac{1}{2m_2} \left[2 \left(\frac{m_2m_3}{Mm_1} \right)^{1/2} r_{23}^2 + \left(\frac{m_1m_3}{Mm_2} \right)^{1/2} (r_{13}^2 + r_{23}^2 - r_{12}^2) \right] \frac{1}{r_{23}} \frac{\delta}{\delta r_{23}}, \\
 K_{22} &= \frac{1}{2M} \left[\frac{m_1}{m_2} r_{13}^2 + \frac{m_2}{m_1} r_{23}^2 + (r_{13}^2 + r_{23}^2 - r_{12}^2) \right] K_0 + \left[\frac{1}{\mu_{12}} r_{13}^2 - \frac{1}{2m_1} (r_{12}^2 + r_{13}^2 - r_{23}^2) \right] \frac{1}{r_{13}} \frac{\delta}{\delta r_{13}} \\
 &\quad + \left[\frac{1}{\mu_{12}} r_{23}^2 - \frac{1}{2m_2} (r_{12}^2 + r_{23}^2 - r_{13}^2) \right] \frac{1}{r_{23}} \frac{\delta}{\delta r_{23}},
 \end{aligned}$$

where

$$M = m_1 + m_2 + m_3,$$

$$\mathbf{r} = \left(\frac{m_1m_3}{Mm_2} \right)^{1/2} (\mathbf{R}_3 - \mathbf{R}_1) + \left(\frac{m_2m_3}{Mm_1} \right)^{1/2} (\mathbf{R}_3 - \mathbf{R}_2), \tag{4}$$

$$\mathbf{P} = \mathbf{R}_2 - \mathbf{R}_1,$$

and the \mathbf{R}_i 's are coordinates of the three particles.

TABLE I. Nonlinear variational parameters used in all s -state wave functions. The parameters are in units of the inverse muon Bohr radius. The values of these parameters suggest the character of a two-center wave function.

a_1	a_2	a_3	b_1	b_2	b_3
0.79	1.24	0.45	0.76	0.441	1.215

TABLE II. Summary of s -state energies in eV with four progressively larger expansions; the last two columns are Bhatia and Drachman's 440-term values and the nonvariational values of Ref. 1, respectively.

	Our calculation			
	230 terms	280 terms	330 terms	380 terms
Ground-state energy	-319.086	-319.094	-319.115	-319.117
Excited-state energy	-34.689	-34.733	-34.772	-34.776
	Bhatia and Drachman			Ref. 1
Ground-state energy		-319.062		-319.15
Excited-state energy		-34.573		-34.87

TABLE III. Nonlinear variational parameters used in a ground p state in units of the inverse muon Bohr radius.

a_1	a_2	a_3	b_1	b_2	b_3
1.2	1.01	0.401	0.871	0.55	1.1

III. RESULTS AND DISCUSSIONS

The mass values used in this calculation are $m_t = 5496.899m_e$, $m_d = 3670.481m_e$, and $m_\mu = 206.7686m_e$.

The nonlinear parameters used in all s states are given in Table I. Our variational energy from four progressively larger expansions are summarized in Table II together with Bhatia and Drachman's value and the nonvariational value of Ref. 1 for comparison. Despite the appearance of excellent agreement (-0.01% discrepancy), the convergence rate for the last two places in the energies (10^{-2} – 10^{-3} eV) is quite slow for both s states. The 230- and 280-term wave functions contain maximum exponents $n_i=6$ where the 330- and 380-term wave functions contain up to $n_i=7$. All s states have the same nonlinear variation parameters. This is not true for the p -state wave functions; however, the nonlinear parameters used in the ground p state are given in Table III. The energies are summarized in Table IV together with the 440-term value from Ref. 2 and the value from Ref. 1. The convergence rate of this state is faster than for any other states. In contrast, the excited p -state converges most slowly. The nonlinear variational parameters are also quite different from those of the ground state. These parameters are listed in Table V. Comparing the nonlinear parameters suggests an excited p state with much larger configuration-space extent. For this state, we have used two different expansions. Slower convergence is obtained if equal numbers of terms are used in f_1 and f_2 . These results are given in Table VI. It is seen that even in this expansion the convergence rate is twice as fast as that of Ref. 2. Faster convergence is achieved when more terms are used in f_1 and a minimum of terms are used in f_2 . f_1 cor-

TABLE IV. Summary of ground p -state energies in eV with four progressively larger expansions. The last two columns are Bhatia and Drachman's 440-term value and the value of Ref. 1, respectively.

Our calculations			
150 terms	200 terms	250 terms	300 terms
-232.417	-232.431	-232.434	-232.436
Bhatia and Drachman		Ref. 1	
-232.416		-232.44	

TABLE V. Nonlinear variational parameters used in the excited p state in units of the inverse muon Bohr radius.

a_1	a_2	a_3	b_1	b_2	b_3
0.557	0.981	0.260	0.557	0.361	0.987

responds to configurations where the two nuclei are in relative p states. f_2 corresponds to configurations where the two nuclei are in a relative s state. Such states contribute very little to the binding energy. They are, however, needed to calculate the sticking probabilities. We have thus included in f_2 those terms which have nonzero derivatives at the coalescence of the two nuclei. Such terms are also needed to satisfy the cusp conditions. The cusp conditions are not built into our present basis functions, however. The results of these expansions are listed in Table VII.

It is seen that even our worst results have discrepancies of less than 2% from that of Ref. 1 and less than 4% from the most recent value.⁴ Our variational energy is very sensitive to the nonlinear parameters a_1 and b_1 . Without them our results would not differ substantially from those of Ref. 2.

IV. CONCLUSIONS

We have demonstrated that it is possible to calculate the weakly bound excited p state of the $(dt\mu)^+$ molecule with our variational method provided proper basis functions are used. There is plenty of room for improvement in our basis functions. An obvious refinement would be a built-in constraint on our basis functions so that the cusp conditions are automatically satisfied. This involves some regrouping of our basis functions. It also results in reducing the dimension of our matrices and hence a faster convergence. Such refinement in our wave functions is obviously advantageous for sticking-coefficient calculations. The precise roles played by the cusp condition and f_2 on the structure of this molecule will be the subject of our subsequent investigation.

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TABLE VI. Excited p -state energy in eV. The variational expansions have an equal number of terms in f_1 and f_2 , respectively. The last two columns are Bhatia and Drachman's 440-term value and the value of Ref. 1, respectively.

Our calculation		Bhatia and Drachman		Ref. 1	
224 terms	300 terms	390 terms			
-0.152	-0.335	-0.437	-0.224		-0.64

TABLE VII. Excited p -state energy in eV with minimum terms in f_2 . The number of terms in f_2 is 150 for the 500-term expansion.

150 terms	225 terms	300 terms	400 terms	500 terms
-0.313	-0.499	-0.563	-0.613	-0.628

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⁴A more recent nonvariational value is -0.656 eV, S. I. Vinitiskii *et al.*, Joint Institute for Nuclear Research, Dubna Report No. P4-84-642 (unpublished).