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Variational calculations of muonic-molecule energy levels

A. K. Bhatia and Richard J. Drachman

Laboratory for Astronomy and Solar Physics, Goddard Space Flight Center, Greenbelt, Maryland 20771 (Received 19 June 1984)

We report the best variational energies obtained to date of the bound states of muonic molecules containing nucleons of unit charge, or isotopes of hydrogen. Hylleraas wave functions are used to describe the three-particle systems, and the convergence of the energies is carefully studied; as many as 440 terms have been included in some cases. These results are compared with the best previous values.

I. INTRODUCTION

The spectra of muonic molecules containing hydrogen isotopes are of renewed interest due to the possibility of realizing useful muon catalyzed fusion.¹ The mass ratios of the particles constituting these molecules are intermediate between those most natural to the Born-Oppenheimer approximation and those for which the Hylleraas type of wave function has been successfully applied in the past. The best previous calculations² have used techniques involving initial description of the systems in terms of Born-Oppenheimer wave functions. These calculations have predicted some very weakly bound excited states, and these, in turn, seem to be very important in the process of μ -molecule formation. It would be useful and interesting to repeat the evaluation of these energy levels using the somewhat more straightforward technique involving three-particle variational trial functions. In this Rapid Communication we carry out this program, recomputing all the bound-state energies of muonic molecules involving ${}^{1}H(p)$, ${}^{2}H(d)$, and ${}^{3}H(t)$, for total angular momentum states 0 and 1. In some cases, the present results prove to be rapidly convergent, and lower energies are obtained here than in any previous calculation. For the most weakly bound levels, however, we obtain binding energies consistent with the previous results, but significantly smaller in magnitude.

II. FORMULATION OF THE PROBLEM

The systems of interest consist of three particles, two nuclei of masses $M_1 \ge M_2$ and positive unit charges, and a negative muon of mass m. It is convenient to write the Hamiltonian of the system in units of the reduced Rydberg of the more massive muonic atom $(R_{\mu_1} = \mu_1/m_e \text{ Ry})$, where the reduced masses are defined, as usual, by $\mu_i = mM_i/(m + M_i)$. Then the Hamiltonian is

$$H = -\vec{\nabla}_{1}^{2} - \left(\frac{\mu_{1}}{\mu_{2}}\right)\vec{\nabla}_{2}^{2} - 2\left(\frac{\mu_{1}}{m}\right)\vec{\nabla}_{1}\cdot\vec{\nabla}_{2} - \frac{2}{r_{1}} - \frac{2}{r_{2}} + \frac{2}{r_{12}} , \qquad (1)$$

where \vec{r}_1 and \vec{r}_2 are the vectors from the muon to the two nucleons. Although there are nine coordinates describing the system, three correspond to the center of mass, and three are Euler angles describing the orientation in space of the triangle whose vertices are the three particles. It is well known that the fundamental dynamical problem can be written in a form involving only the three interparticle distances r_1 , r_2 , and r_{12} . We use the symmetric Euler-angle method³ to carry out this reduction; although most natural for the case of identical nucleons $(M_1 = M_2, \text{ i.e., } p\mu p, d\mu d, \text{ and } t\mu t)$, it can also be readily applied to nonidentical cases. We will be concerned here with total angular momenta J = 0 and 1 and parities $(-1)^J$; the corresponding wave functions have the following forms:

$$\Psi_{J=0} = (f+g)\mathcal{D}_0^{0+} ; \qquad (2)$$

$$\Psi_{J=1} = -\cos(\theta_{12}/2)(f+g)\mathcal{D}_1^{1+} - \sin(\theta_{12}/2)(f-g)\mathcal{D}_1^{1-} .$$

For nonidentical nucleons, both functions
$$f$$
 and g have



FIG. 1. Binding energy of the molecule $d\mu d$ for both J = 1 states. The difference between the binding energy B(N) and the asymptotic binding energy $B(\infty)$ [Eq. (5)] is plotted against the expansion length N. The Pekeris numbers corresponding to the plotted points run from $\Omega = 4(N = 35)$ to $\Omega = 11(N = 364)$. The smooth curves are interpolations to guide the eye.

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similar forms:

$$\begin{cases} f \\ g \end{cases} = e^{-(\gamma r_1 + \delta r_2)} \binom{r_1}{r_2}^J \sum_{l,m,n \ge 0} C(l,m,n) r_1^l r_2^m r_{12}^n , \qquad (3)$$

but the parameters need not be the same. For identical nucleons, the symmetry imposes the relation

$$r(r_1, r_2, r_{12}) = (-1)^J f(r_2, r_1, r_{12}) \quad . \tag{4}$$

The rotational harmonics (\mathscr{D}) appearing in Eq. (2) have been defined in Ref. 3, and the detailed form of the kinetic-energy operator also appears there. The calculations reported here are of the conventional Rayleigh-Ritz variational type, although we paid particular attention to optimizing the nonlinear parameters.

At first sight, our choice of trial functions [Eq. (3)] does not seem particularly useful. Although the motion of the muon, relative to the heavy particles, should be well described by the powers and exponentials of r_1 , r_2 , and r_{12} appearing there, the relative motion of the two nucleons might seem to call for a "molecular" type of wave function. Nevertheless, it seemed worthwhile to carry out a straightforward calculation with the present type of function extended to as great an expansion length N as possible. For modest values of N, the usual numerical techniques for diagonalization were satisfactory, but they began to fail for N > 120. In order to continue our investigation to higher values of N, we used the method of inverse iteration;⁴ this technique enabled us to use expansion lengths of up to 440 terms.

In this method, one uses a preliminary estimate E_0 of the eigenvalue being sought, in effect constructs the operator $(H-E_0)^{-1}$ and iterates until only the largest eigenvalue of the inverse operator remains; this process isolates the energy eigenvalue closest to E_0 . In favorable cases, this energy can be evaluated to at least ten significant figures. In all the cases reported, however, convergence was obtained to the number of significant figures shown.

III. RESULTS

As might be expected, the low-lying states of each species and each value of the angular momentum are easier to treat, while the weakly bound excited states converge more slowly. To illustrate this, we have plotted the binding energies of the lowest p state (J = 1, v = 0) and the excited pstate (J = 1, v = 1) for the symmetrical case $d\mu d$ as functions of N, relative to an estimated asymptotic value (Fig. 1). It can be seen that the convergence is much better in the former case than in the latter. To obtain such an asymptotic estimate for the energy, one compares the variational energies obtained for the three largest expansions calculated, corresponding to three successive Pekeris numbers. [We follow the tradition of reporting results only at certain

TABLE I. Binding energies in eV for all the muonic hydrogen isotopic molecules for angular momentum J = 0, 1. For each species, the first line is our best value, the second line in parentheses, is the maximum number of terms retained, the third line, in square brackets, is the extrapolated asymptotic value from Eq. (5), and the fourth line is from Ref. 2. (We used the following values of the constants: $M_p = 1836.151m_e$, $M_d = 3670.481m_e$, $M_t = 5496.899m_e$, $m = 206.7686m_e$, 1 Ry = 13.605 804 eV. All of these have fractional errors of about 10^{-6} , in some case leading to meV errors in the tabulated binding errors as indicated by subscripts.)

Species	J=0, v=0	J = 0, v = 1	J=1, v=0	J=1, v=1
	253.15 ₂		107.266	
рμр	(125)		(286)	
	[253.153]		[107.26 ₆]	
	252.95		106.96	
pµd	221.54 ₁		97.493	
	(440)		(440)	
	[221.561]		[97.493]	
	221.52		97.40	
	213.829		99.119	
pμt	(440)		(440)	
- •	[213.857]		[99.119]	
	213.97		99.01	
dµd	325.07 ₀	35.815	226.662	1.862
	(203)	(161)	(286)	(364)
	[325.083]	[35.846]	$[226.68_0]$	[1.87]
	325.04	35.80	226.61	1.91
dµt	319.06 ₂	34.573	232.41 ₆	0.224
	(440)	(440)	(440)	(440)
	[319.25]	• • •	[232.41 ₆]	
	319.15	34.87	232.44	0.64
	362.90 ₀	83.630	289.12 ₀	45.096
t µ t	(203)	(161)	(286)	(286)
	[362.945]	[83.67]	[289.12]	[45.187]
	362.95	83.88	289.15	45.24

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values of N; these correspond to including all exponents l,m,n in Eq. (3) such that $l+m+n \leq \Omega$, where the integer Ω is called the Pekeris number.] The assumption that the energy converges geometrically, i.e., that $E(\Omega + 1) - E(\Omega) = cp^{\Omega}$ implies an asymptotic value of the energy given by

$$E(\infty) = \frac{[E(\Omega+1)]^2 - E(\Omega)E(\Omega+2)}{2E(\Omega+1) - E(\Omega) - E(\Omega+2)} \quad .$$
 (5)

In Table I, we show all the binding energies we have computed so far, including the interesting weakly bound excited J = 1 states of $d\mu d$ and $d\mu t$. It is clear that the present method is very accurate for some of these systems, yielding better values for the binding energies in some cases than those of Ref. 2. In other cases, especially those involving unsymmetrical molecules where two independent functions appear in Eq. (2), our computational ability is exhausted before full convergence is achieved. Further work, involving

- ¹L. Bracci and G. Fiorentini, Phys. Rep. **86**, 169 (1982); S. E. Jones *et al.*, Phys. Rev. Lett. **51**, 1757 (1983).
- ²S. I. Vinitskii *et al.*, Zh. Eksp. Teor. Fiz. **79**, 698 (1980) [Sov. Phys. JETP **52**, 353 (1980)].
- ³A. K. Bhatia and A. Temkin, Rev. Mod. Phys. **36**, 1050 (1964); Phys. Rev. **137**, A1335 (1965).
- ⁴J. H. Wilkinson, *The Algebraic Eigenvalue Problem* (Oxford Univ. Press, London, 1965), p. 570.

rearrangement or optimization of the trial functions, will be undertaken later. [In all comparable cases, the present results exceed the variational results of Carter;⁵ e.g., for $p \mu p$ by 0.06 eV and for $d \mu d$ (v = 1) by 3.05 eV.]

With these rather sophisticated wave functions it should eventually be possible to compute fusion rates and sticking probabilities,¹ which involve the point of coalescence of the two nucleons.⁶ So far, no reliable results for these important quantities have been obtained, since the region of coalescence is not necessarily well represented in a function designed to minimize the energy. Use of global operator identities⁷ and cusp conditions⁸ may help.

Note added in proof. Using a variational method with up to 375 exponential basis functions, A. M. Frolov and V. D. Efros [Pis'ma v Zh. E. T. F. **39**, 449 (1984)] have recently calculated binding energies for the same states discussed above. In most cases they are comparable to or better than ours, while in three cases our results are better.

- ⁵B. P. Carter, Phys. Rev. 165, 139 (1968).
- ⁶B. P. Carter, Phys. Rev. 141, 863 (1966).
- ⁷J. Hiller, J. Sucher, and G. Feinberg, Phys. Rev. A **18**, 2399 (1978); H. P. Trivedi, J. Phys. B **13**, 839 (1980); R. J. Drachman, *ibid.* **14**, 2733 (1981).
- ⁸T. Kato, Commun. Pure Appl. Math. **10**, 151 (1957); R. T. Pack and W. B. Brown, J. Chem. Phys. **45**, 556 (1966).