

Accurate solution method in the three-body problem and binding energies of mesic molecules

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An effective method for very accurately solving three-body atomic and molecular problems is proposed. The existence of weakly bound $dd\mu^*$ and $dt\mu^*$ systems with $L = 1$ is established rigorously. The binding energies of these mesic molecules are calculated with an accuracy sufficient for μ catalysis. The binding energies of other μ molecules of hydrogen isotopes are also calculated.

The observation that $dd\mu$ and $dt\mu$ molecules form rapidly at certain temperatures has reattracted interest to the μ catalysis of fusion reactions.¹ These high formation rates are attributed to a resonant mechanism for the formation of these molecules,² which involves hypothesized weakly bound $L = 1$ states of these molecules.³ Such states have been found in calculations at Dubna,⁴ but not in many other calculations.³ The nonvariational method of Ref. 4 involves some subtle points, and it is difficult to thoroughly analyze its accuracy. It would be preferable to solve the problem by a more direct method, as Vinnitskiĭ *et al.*⁴ themselves pointed out. A quantitative description of the temperature dependence of the production of $dd\mu$ and $dt\mu$ molecules requires a prediction of the positions of their weakly bound levels with an accuracy of 10^{-2} – 10^{-3} eV. This accuracy corresponds to an extremely small value in terms of the characteristic units of the problem, so that the relative accuracy required of the solution of the problem is³ 10^{-6} . This accuracy has essentially not been achieved by the methods available.³

We denote by \mathbf{r}_1 and \mathbf{r}_2 the coordinates of the nuclei, while \mathbf{r}_3 is the coordinate of the μ^- meson. We adopt the following representation for the wave function of the three-body system:

$$\psi = \sum_{l=0}^L \sum_i C_l^{(i)} Y_{LM}^{l_i} r_{LM}^{-l}(\mathbf{r}_{13}, \mathbf{r}_{23}) \exp(-\alpha_1^{(i)} r_{23} - \alpha_2^{(i)} r_{13} - \alpha_3^{(i)} r_{23}), \quad (1)$$

where

$$Y_{LM}^{l_1 l_2}(\mathbf{x}, \mathbf{y}) = x^{l_1} y^{l_2} [Y_{l_1 m_1}(\mathbf{n}_x) Y_{l_2 m_2}(\mathbf{n}_y)]_{LM}.$$

The parity of ψ is obviously $(-1)^L$; for the $(-1)^{L+1}$ parity, the corresponding expansion contains $Y_{LM}^{l_1 l_2}(\mathbf{r}_{31}, \mathbf{r}_{32})$ with $1 \leq l \leq L$. Expansion (1) generalizes to arbitrary states some approaches which have been taken previously for $L = 0$ and also in the special case of Refs. 5 and 6. Expansion (1) converges extremely rapidly for the ground states, actually faster than in the case of a basis of polynomials in r_{ij} of the Hylleraas type; for weakly bound states the difference in convergence rates is even greater since the number of exponential functions required in (1) does not increase significantly with

increasing clustering. An important point is that it is not necessary to choose exponential functions. If we were to arbitrarily write

$$\psi(r) = \int d\alpha \psi(\alpha) \exp(-\alpha r) = \sum_{i=1}^N c_i \exp(-\alpha_i r) \quad (2)$$

then for any "sufficiently reasonable" distribution of arguments α_i the accuracy of the results would increase rapidly with increasing N and would depend only weakly on the details of their distribution. We have selected these arguments as follows: $\alpha_{ij}^{(i)} = t_{ij} A_j$, where (in mesic-atom units) $A_1 = A_2 = 1.5$, $A_3 = 2$; $t_{ij} = \langle \frac{1}{2} i(i+1)\sqrt{n_j} \rangle$, $\langle \dots \rangle$ where the angle brackets denote the fractional part of the number, and $n_1 = 2$, $n_2 = 3$, and $n_3 = 5$. For the $d\mu^*$ system we have $A_1 = 1.25$, $A_2 = 1.05$, and $A_3 = 1.45$. A similar choice was used in Ref. 5, but with excessive complications; that choice corresponds to a certain method for converting a three-dimensional integral of the type in (2) into discrete form.

Simple analytic expressions have been derived for all the matrix elements of the problem in basis (1). These expressions are polynomials of the quantities

$$X_p = (\alpha_{ql}^{(i)} + \alpha_{rl}^{(i)} + \alpha_{ql}^{(i')} + \alpha_{rl}^{(i')})^{-1},$$

where $p, q, r = 1, 2, 3$. After a spatial averaging, the calculations are carried out in parametric coordinates. Simple analytic expressions cannot be derived by the conventional approaches which use D functions of three partial Euler angles, Y_{LM}^{L-L} , $Y_{LM}^{L+L+1-L}$, which, like these D functions, form a complete system of angular wave functions.⁷ In the case of the $pp\mu$, $dd\mu$, and $tt\mu$ systems, a symmetrization (or antisymmetrization) of the basis functions from (1) leads to the condition $l \geq L/2$, reducing the number of these functions.

Table I lists the binding energies $-\epsilon_L(N_i)$, in electron volts, calculated by this method for the ground and excited states of mesic molecules with $L = 0$ and $L = 1$; here N_i is the number of basis wave functions from (1) which are taken into account. These wave functions form a complete system, and in the limit $N \rightarrow \infty$ the energies $-\epsilon_L(N)$ approach the actual energies arbitrarily closely. The convergence rate can be seen in Table I. For homonuclear systems with $L = 0$ we use $N_1 = 100$, $N_2 = 125$, and $N_3 = 140$; for the $d\mu^*$ system with $L = 1$ we use $N_1 = 250$, $N_2 = 300$, and $N_3 = 375$; in the other cases we use $N_1 = 125$, $N_2 = 200$, and $N_3 = 250$. The results on $-\epsilon_L(N)$ conform to smooth curves, which can be extrapolated to $-\epsilon_L(\infty)$, and the later values are also listed in Table I. For the values of $-\epsilon_L(\infty)$ we have retained those signs which can be assumed correct. We used the constant values $R_y = 13.6058041$ eV, $m_p = 1836.151527$, the values of $m_{d,t,\mu}$ from Refs. 3 and 4, $E(p\mu) = -2528.52171$ eV, $E(d\mu) = -2663.23087$ eV, and $E(t\mu) = -2711.27278$ eV.

As a control we solved the problem of the ground state of the ${}^\infty\text{He}$ atom. We found $E(139) = -2.9037243135$ a.u. and $E(\infty) = -2.90372437$ a.u., in agreement with the known exact result to all the places shown.

The variational results on $-\epsilon_L(N_i)$ shown in Table I were obtained by diagonalizing the Hamiltonian matrix, so that all these results are lower limits on the actual

TABLE I.

	$pp\mu$	$dd\mu$	$tt\mu$	$dd\mu^*$	$tt\mu^*$	$dpp\mu$	$tp\mu$	$dtt\mu$	$dt\mu^*$
$-\epsilon_{L=0}(N_1)$	253.15040	325.06695	362.87101	35.69446	83.54017	221.53393	213.82847	319.04991	34.34204
$-\epsilon_{L=0}(N_2)$	253.15205	325.07124	362.89558	35.81093	83.68414	221.54781	213.83896	319.13451	34.79112
$-\epsilon_{L=0}(N_3)$	253.15240	325.07213	362.90040	35.83658	83.72202	221.54923	213.83975	319.13805	34.82381
$-\epsilon_{L=0}(\infty)$	253.153	325.074	362.904	35.9	83.78	221.551	213.841	319.140	34.84
$-\epsilon_{L=1}(N_1)$	107.24811	226.66621	289.10278	-0.02433	44.99089	96.70044	98.28906	231.56104	0.26650
$-\epsilon_{L=1}(N_2)$	107.26398	226.68014	289.13344	1.64231	45.16918	97.32169	99.05239	232.34977	0.45129
$-\epsilon_{L=1}(N_3)$	107.26563	226.68157	289.13931	1.78123	45.19359	97.42990	99.10104	232.42049	0.52310
$-\epsilon_{L=1}(\infty)$	107.267	226.683	289.146	1.95 ± 0.05	45.22	97.66	99.13	232.48	0.6

values, in accordance with the well-known theorems.⁸ Consequently, the fact that we find positive values for $-\epsilon_{L=1}(N_i)$ for the $dd\mu^*$ and $dt\mu^*$ systems is rigorous proof that these important states exist. The results for these systems agree satisfactorily with the results found in Ref. 4 (the latter are not lower limits on the actual values).

These mesic-molecule results are the most accurate to be published (the number of correct digits in the values in Table I is the highest³; another measure of the accuracy for variational calculations is the absolute value of the energy minimum⁸). The wave functions constructed here, (1), have an extremely simple structure and are convenient for applications. The method described here is the most effective one for solving a broad range of three-body problems.

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