THE GROUND STATE OF THE (p–μ–p)$^+$ MOLECULE ION

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Summary

This paper gives the results of a variational calculation using a 100-term wavefunction on the ground (para) state of (p–μ–p)$^+$, including the effects of the finite proton mass. The energy found is sensitive to the muon mass; with $m_\mu = 206\cdot77\, m_e$, we find (B.E.)$_{p\mu p}$ to be $253\cdot14 \pm 0\cdot01$ eV. Results are also given for the muon–proton overlap, and for a number of other geometric averages of the wavefunction.

I. Introduction

The stable Coulombic bound system (p–μ–p)$^+$ is of some importance in the analysis of muon capture experiments and a number of calculations have previously been performed on both the ground state ($L = 0$) and first excited state ($L = 1$). The earlier calculations (Cohen, Judd, and Riddell 1960; Ta-You Wu, Rosenberg, and Sandstrom 1960) were limited in accuracy by their use of the Born–Oppenheimer approximation, while later calculations (Kalos, Roothaan, and Sack 1960; Halpern 1964; Wessel and Phillipson 1964; Kabir 1966) have retained the full (non-relativistic) Hamiltonian. We discuss here a series of variational calculations on the ground state using the full Hamiltonian and retaining up to 100 terms in the wavefunction. Values are given for the energy, for the muon–proton overlap γ (which is of interest in non-capture), and for some 50 other geometric averages over the p–μ–p wavefunction. The results are in agreement where applicable with those of Wessel and Phillipson (1964).

II. Method

Let $\mathbf{r}_1$ and $\mathbf{r}_2$ be the position vectors of the two protons relative to the muon and let $r_1 \equiv |\mathbf{r}_1|$, $r_2 \equiv |\mathbf{r}_2|$, and $r_{12} \equiv |\mathbf{r}_1 - \mathbf{r}_2|$. We then define the operators

$$T_0 \equiv \nabla_1^2 + \nabla_2^2, \qquad T_{12} \equiv \nabla_1 . \nabla_2, \qquad T_\infty \equiv T_0 + 2T_{12}.$$

Then the total kinetic energy operator T becomes

$$\begin{aligned} T &= -(\hbar^2/2m_{\rm red})T_0 - (\hbar^2/m_\mu)T_{12} \\ &= -(\hbar^2/2m_\mu)T_\infty - (\hbar^2/2m_{\rm p})T_0, \end{aligned}$$

with

$$m_{\rm red} \equiv m_\mu m_{\rm p}/(m_\mu + m_{\rm p}).$$

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The ground state wavefunction of $(\mathrm{p}-\mu-\mathrm{p})^+$ is a function only of the interparticle distances r_1, r_2, and r_{12}. We take a trial function of the form

$$\psi_T = \sum_{i=1}^{N} a_i(1+P_{12})\exp[-\alpha^{-1}\{Z^*(l_i r_1 + m_i r_2)+n_i r_{12}\}], \tag{1}$$

where P_{12} is the permutation operator, the a_i are a set of linear parameters, α and Z^* are nonlinear parameters, and (l_i, m_i, n_i) are a triplet of integers that are ordered in a systematic way such that the following conditions are all satisfied:

$$\left.\begin{array}{ll}\text{(i)} & l_i \geqslant m_i\,, \\ \text{(ii)} & n_i \geqslant n_{\min}\,, \\ \text{(iii)} & \text{the Hamiltonian is Hermitian with respect to } \psi_T, \\ \text{(iv)} & \text{the possible values of } q\ (= l_i+m_i+n_i) \text{ are} \\ & \text{successively exhausted.}\end{array}\right\} \tag{2}$$

Condition (iii) merely excludes values of l, m, and n for which the wavefunction is not normalizable.

The programme incorporating this wavefunction will be described in detail elsewhere (Delves and Kalotas, in preparation) together with the reasons for the above choice of basis functions; here we quote only the results obtained for the system p–μ–p. For these calculations we have set

$$Z^* = 1\,, \qquad n_{\min} = -1\,, \tag{3}$$

and have varied the scale factor α for values of N up to 100.

The energy E depends on the value assumed for the muon mass m_μ. We shall quote results in muon atomic units and in electron-volts. We take

$$m_\mu = 206\cdot77\, m_{\mathrm{e}}\,, \qquad m_{\mathrm{p}} = 1836\cdot12\, m_{\mathrm{e}}\,. \tag{4}$$

We have 1 $(\mathrm{a.u.})_{\mathrm{e}} = 27\cdot2098$ eV and hence

$$1\ (\mathrm{a.u.})_\mu \equiv \mathrm{a}_\mu = 5626\cdot1703\ \mathrm{eV}. \tag{5}$$

III. Results

The dependence of the upper bounds $E(N)$ on α for various values of N is shown in Figure 1, while optional values of α and energies E are given in Table 1. In this table the binding energy is the energy by which the last proton is bound

$$\begin{aligned}\mathrm{B.E.} &= -\{E - E(\mathrm{p}\mu)\} \\ &= -E - 0\cdot5(m_{\mathrm{red}}/m_\mu)\,\mathrm{a}_\mu = -E - 2528\cdot360\ \mathrm{eV}\,,\end{aligned} \tag{6}$$

with m_{red} defined as above. The best result from Table 1, B.E. $\geqslant 253\cdot133$ eV, should be compared with the value B.E. $\geqslant 254\cdot3$ eV obtained by Wessel and

Phillipson (1964). Their assumed value for the muon mass, although not stated explicitly, appears from the value for $E(p\mu)$ quoted there to be

$$m_\mu = 206 \cdot 8\, m_e\,. \tag{7}$$

The mass m_μ affects the quoted energy not only through the conversion constant from muon atomic units to electron volts, but also through the term in the Hamiltonian coming from the finite size of m_μ/m_p (see Section II).

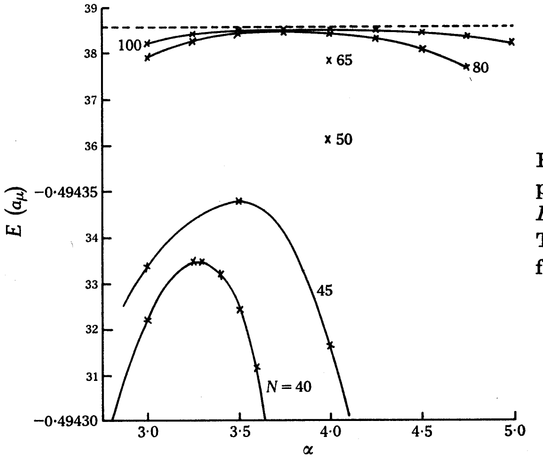

Fig. 1.—The dependence on the scale parameter α of the upper bounds $E(N)$ for various numbers of terms N. The dashed line is the estimated limit for $N \to \infty$.

TABLE 1

OPTIONAL VALUES OF SCALE FACTOR α AND ENERGY E FOR VARIOUS NUMBERS OF TERMS N IN THE WAVEFUNCTION (1)

N	α	Energy E (a_μ)	E (eV)	B.E. (eV)
40	3·3	−0·49433500	−2781·2129	+252·853
45	3·5	−0·49434780	−2781·2849	+252·925
80	3·75	−0·49438441	−2781·4909	+253·1306
100	3·75	−0·49438482	−2781·4932	+253·1329

We have evaluated the expected values of the operators T_0 and T_{12} separately (see Section IV) and hence can correct for the effect of small changes in the assumed muon mass. Using the expected value of T_∞ $(= T_0 + 2T_{12})$ from Section IV we find

$$\begin{aligned}\text{B.E.}\{m_\mu(1+\delta)\} &= \text{B.E.}(m_\mu) + [\{m_p/(m_p+m_\mu)\}E(p\mu) - \tfrac{1}{2}T_\infty]\delta \quad a_\mu \\ &= \text{B.E.}(m_\mu) + 145 \cdot 67\,\delta \quad \text{eV}\,. \end{aligned} \tag{8}$$

This yields, for comparison with Wessel and Phillipson, the value

$$\text{B.E.} = 253 \cdot 15\ \text{eV}\,, \qquad m_\mu = 206 \cdot 8\,. \tag{9}$$

We are unable to explain this discrepancy. We have analysed the rate of convergence of our expression by taking runs for a fixed value of $\alpha = 4 \cdot 0$. The result of these runs is shown below:

N	40	45	50	65
E	$-0\cdot49420763$	$-0\cdot49431666$	$-0\cdot49436131$	$-0\cdot49437836$

N	80	100	∞
E	$-0\cdot49438403$	$-0\cdot49438480$	$-0\cdot4943855$

If we assume the convergence to be of the form (Schwartz 1963)

$$E(N) = E_\infty + AN^{-p}, \tag{10}$$

then these results imply that

$$p = 8 \qquad \text{and} \qquad E_\infty = 0\cdot4943855 \pm 0\cdot075\,. \tag{11}$$

Since extrapolation of this kind is notoriously difficult, we increase the error estimate by a factor of three and quote as our final result for the binding energy

$$253\cdot13 \leqslant \text{B.E.} \leqslant 253\cdot15 \text{ eV} \quad (m_\mu = 206\cdot77)\,. \tag{12}$$

TABLE 2

RESULTS FOR OPERATORS IN THE GROUND STATE OF p–μ–p AS A FUNCTION OF THE NUMBER OF TERMS RETAINED IN THE TRIAL FUNCTIONS

The last column gives the estimated value for $N \to \infty$. All results are in muon units a_μ

Operator	Number of Terms N					
	40	50	65	80	100	∞
T_0	$-1\cdot144820$	$-1\cdot145259$	$-1\cdot146442$	$-1\cdot146982$	$-1\cdot147014$	$-1\cdot1470$
T_{12}	$-0\cdot142563$	$-0\cdot142969$	$-0\cdot143453$	$-0\cdot143688$	$-0\cdot143706$	$-0\cdot1437$
T_∞	$-0\cdot859695$	$-0\cdot859320$	$-0\cdot859536$	$-0\cdot859606$	$-0\cdot859603$	$-0\cdot85960$
$r_1^{-1}+r_2^{-1}$	$1\cdot340478$	$1\cdot340244$	$1\cdot340491$	$1\cdot340603$	$1\cdot340602$	$1\cdot3406$
r_{12}^{-1}	$0\cdot351835$	$0\cdot351737$	$0\cdot351793$	$0\cdot351832$	$0\cdot351831$	$0\cdot35183$
r_1+r_2	$4\cdot773050$	$4\cdot773697$	$4\cdot772134$	$4\cdot771302$	$4\cdot771331$	$4\cdot7713$
$r_1^2+r_2^2$	$15\cdot547886$	$15\cdot555133$	$15\cdot543640$	$15\cdot538348$	$15\cdot538789$	$15\cdot5385$
r_{12}	$3\cdot301826$	$3\cdot301657$	$3\cdot300229$	$3\cdot299493$	$3\cdot299494$	$3\cdot2995$
$\delta(r_1)+\delta(r_2)$	$0\cdot264562$	$0\cdot262824$	$0\cdot262840$	$0\cdot262859$	$0\cdot263041$	$0\cdot2628$
$\delta(r_{12})$	$10\cdot83\times10^{-5}$	$8\cdot22\times10^{-5}$	$4\cdot62\times10^{-5}$	$3\cdot86\times10^{-5}$	$3\cdot96\times10^{-5}$	$4\cdot0\times10^{-5}$

IV. EXPECTED VALUES OF OPERATORS

We have also calculated the expected values of a number of simple operators. These operators include:

(1) the delta function operators $\delta(r_1)+\delta(r_2)$ and $\delta(r_{12})$;

(2) the three kinetic energy terms T_0, T_{12}, and T_∞ defined in Section II;

(3) the potential terms $(r_1^{-1}+r_2^{-1})$ and r_{12}^{-1}, and mean radii r_1+r_2, $r_1^2+r_2^2$, and r_{12}.

The results found for these operators are given in Table 2 as a function of the number of terms N retained. All values are expressed in muon units a_μ. The last column in this table gives an estimate of the extrapolated value for $N \to \infty$.

The estimated accuracy is shown by the number of digits retained; in each case, the last digit shown may be in error by one or two units. Especially noteworthy is the result obtained for $\delta(r_{12})$. The expected value of this operator is zero in the Born–Oppenheimer approximation, and the small value and slow convergence obtained is a consequence of this.

We have also calculated the expected values of various powers of the interparticle distances

$$\langle l, m, n\rangle = \langle\psi \mid (r_1^l r_2^m + r_2^l r_1^m) r_{12}^n \mid \psi\rangle .$$

The extrapolated results for these operators are given in Table 3; again, the estimated accuracy is indicated by the number of digits retained.

TABLE 3

EXPECTED VALUES OF POWERS OF THE INTERPARTICLE DISTANCES

Extrapolated results are for operators of the form $(l, m, n) \equiv (r_1^l r_2^m + r_2^l r_1^m) r_{12}^n$. All values are in muon units a_μ

l	m	n	Value	l	m	n	Value	l	m	n	Value
−1	−1	−1	0·33116	−1	1	0	3·5684	1	1	1	39·248
−1	0	−1	0·50982	−1	2	0	12·2001	−1	−1	2	6·5302
−1	1	−1	1·17052	−1	3	0	49·972	−1	0	2	14·7993
−1	2	−1	3·4930	0	3	0	63·09	−1	1	2	50·929
−1	3	−1	12·651	1	1	0	10·342	−1	2	2	221·67
0	1	−1	1·51753	1	2	0	31·71	0	0	2	24·7808
0	2	−1	4·4328	−1	−1	1	2·05008	0	1	2	70·645
0	3	−1	16·171	−1	0	1	4·15208	−1	−1	3	23·8050
1	1	−1	3·1146	−1	1	1	12·6270	−1	0	3	59·801
1	2	−1	8·869	−1	2	1	48·905	−1	1	3	231·3
1	3	−1	32·31	−1	3	1	224·5	0	0	3	104·54
2	2	−1	24·776	0	1	1	17·261				
−1	−1	0	0·75094	0	2	1	62·306				

Results for the operators $\delta(r_1)+\delta(r_2)$ and r_{12} have been given previously by Wessel and Phillipson (1964), who calculated the muon–proton overlap γ defined by

$$\gamma = \tfrac{1}{2}\pi\langle\delta(r_1)+\delta(r_2)\rangle . \tag{13}$$

In terms of the units used by them ($m_{\text{red}} = 1$) we find

$$\left.\begin{aligned} \gamma &= 0\cdot5686 \quad (0\cdot5733), \\ \langle r_{12}\rangle &= 2\cdot9655 \quad (2\cdot973), \end{aligned}\right\} \tag{14}$$

where the results of Wessel and Phillipson are given in parentheses. In both cases, the present results agree within the accuracy ($\sim 1\%$) claimed by Wessel and Phillipson.

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