than 3% of the quadratic shift. However, the transition observed is unsuitable for revealing a possible breakdown of parity or electron electric dipole moment, since $\Delta m_F = 0$.

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†Now at the University of Washington, Seattle, Washington.

‡Alfred P. Sloan Fellow.

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QUANTUM MECHANICS OF THE $(p\text{-}\mu\text{-}p)^+$ MOLECULAR ION*

W. Roy Wessel
Department of Physics, University of Michigan, Ann Arbor, Michigan

and

Paul Phillipson
Department of Physics, University of Colorado, Boulder, Colorado

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Two protons and a μ^- meson can form a Coulombically stable three-body system in the ground (para) state similar to the ground state of its molecular prototype H_2^+. The first stable excited state of $(p\text{-}\mu\text{-}p)^+$ (ortho state) has a total angular momentum of one quantum unit and corresponds roughly to the first rotationally excited state of H_2^+.[1] Electronic wave functions for H_2^+ can be found[2] to within an error on the order of $M_e/M_p = 0.0005$ in the Born-Oppenheimer approximation[3] but analogous calculations for $(p\text{-}\mu\text{-}p)^+$ have inherent errors on the order of $M_\mu/M_p = 0.1$. It is desirable to have $(p\text{-}\mu\text{-}p)^+$ wave functions which are free of this error, not only because of the intrinsic interest of the problem but also because of recent muon capture experiments, such as those of Rothberg et al.,[4] whose interpretation ultimately depends upon accurate knowledge of $(p\text{-}\mu\text{-}p)^+$ wave functions. We have computed wave functions and energies using the exact Hamiltonian of $(p\text{-}\mu\text{-}p)^+$ and have not invoked the Born-Oppenheimer approximation, although the spin of the particles is neglected here.

Eliminating the three coordinates of the center of mass leaves a wave equation in 6 space variables. Since $(p\text{-}\mu\text{-}p)^+$ can be viewed as a moleculelike system, one useful choice of coordinates is the three Euler angles (α, β, γ) and internal coordinates (ρ, ξ, η). The three particles define a triangle, shown in Fig. 1, whose orientation with respect to some inertial coordinate system moving with the center of mass is given by (α, β, γ) and whose shape is given by (ρ, ξ, η). The internal coordinates are related to the interparticle distances by

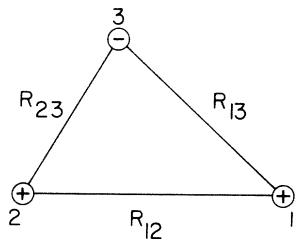

FIG. 1. $(p\text{-}\mu\text{-}p)^+$ system showing interparticle coordinates. The μ^- particle is taken as particle 3.

$$\rho = R_{12},$$

$$\xi = (R_{23} + R_{13})/R_{12},$$

$$\eta = (R_{23} - R_{13})/R_{12}.$$

The Hamiltonian, similar to that of Wu, Rosenberg, and Sandstrom,[5] can be written in terms of these variables as $H = H_0 + H_1 + H_2$, where

$$H_0 = -\frac{2}{\rho^2(\xi^2-\eta^2)}\left[\frac{\partial}{\partial\xi}(\xi^2-1)\frac{\partial}{\partial\xi} + \frac{\partial}{\partial\eta}(1-\eta^2)\frac{\partial}{\partial\eta} + \left(\frac{1}{\xi^2-1}+\frac{1}{1-\eta^2}\right)\frac{\partial^2}{\partial\gamma^2}\right] + \frac{1}{\rho}\left[-\frac{2}{\xi+\eta}-\frac{2}{\xi-\eta}+1\right],$$

$$H_1 = -\frac{m_\mu}{m_p}\frac{1}{\rho^2}\left\{-\vec{K}^2(\alpha,\beta,\gamma) + \frac{\partial}{\partial\rho}\rho^2\frac{\partial}{\partial\rho} - 2\frac{\partial^2}{\partial\gamma^2} - \frac{2}{(\xi^2-\eta^2)}\left[(\xi^3-\xi)\frac{\partial}{\partial\xi} + (\eta-\eta^3)\frac{\partial}{\partial\eta}\right]\left(1+\rho\frac{\partial}{\partial\rho}\right)\right.$$
$$\left. + \frac{\xi^2+\eta^2}{\xi^2-\eta^2}\left[\frac{\partial}{\partial\xi}(\xi^2-1)\frac{\partial}{\partial\xi} + \frac{\partial}{\partial\eta^2}(1-\eta^2)\frac{\partial}{\partial\eta} + \left(\frac{1}{\xi^2-1}+\frac{1}{1-\eta^2}\right)\frac{\partial^2}{\partial\gamma^2}\right]\right\},$$

$$H_2 = \frac{m_\mu}{m_p}\frac{1}{\rho^2}\left\{\frac{2\xi\eta}{[(\xi^2-1)(1-\eta^2)]^{1/2}}iK_{x'}(\alpha,\beta,\gamma)\frac{\partial}{\partial\gamma} + 2\frac{[(\xi^2-1)(1-\eta^2)]^{1/2}}{(\xi^2-\eta^2)}iK_{y'}(\alpha,\beta,\gamma)\left[\xi\frac{\partial}{\partial\eta} - \eta\frac{\partial}{\partial\xi}\right]\right\}.$$

The Hamiltonian has been made dimensionless by choosing the unit of length to be the Bohr radius, $a_\mu = \hbar^2/M_\mu e^2$, and the unit of energy to be e^2/a_μ. $\vec{K}$ is the total angular momentum operator,[6] and two operators which commute with this Hamiltonian are $\vec{K}^2$ and $K_z = -i\partial/\partial\alpha$. Thus the eigenfunctions of H can be chosen to be eigenfunctions of these operators as well.

The Euler angles can be eliminated from the Hamiltonian by expanding the wave function in terms of the eigenfunctions of the symmetric top,[7] i.e.,

$$\psi_m^{(K)} = \sum_{\lambda=-K}^{K} D_{m,\lambda}^{(K)}(\alpha,\beta,\gamma)\Phi_\lambda^{(K)}(\rho,\xi,\eta).$$

Substituting this expansion into the Hamiltonian reduces it to a set of $(2K+1)$ equations in ρ, ξ, and η alone. Thus for the para state $(K=0)$ we have a single equation $H\Psi(\rho,\xi,\eta) = E\Psi(\rho,\xi,\eta)$. An approximate solution of this equation can be obtained by expanding Ψ in terms of a suitable basis set and obtaining a matrix equation for the coefficients by the Rayleigh-Ritz variational technique.[8] One such set is a generalization of that used by Fröman and Kinsey[9] for the same type of calculation, the power series basis set:

$$\{\rho^r\xi^q\eta^p \exp[-\tfrac{1}{2}\rho\xi - \tfrac{1}{2}\delta^{-2}(\rho-\rho_0)^2]\},\quad r \geq q+p\ (p \text{ even}).$$

A second choice is an orthogonal polynomial basis set

$$\{\rho^r L_q(\rho\xi-\rho)P_p(\eta)\exp[-\tfrac{1}{2}\rho\xi - \tfrac{1}{2}\delta^{-2}(\rho-\rho_0)^2]\},$$
$$r \geq p\ (p \text{ even}),$$

where L_q is the qth simple Laguerre polynomial, and P_p is the pth Legendre polynomial. This latter basis set was chosen for the functional independence of its terms which tends to prevent ill-conditioning of the matrix,[9] and its use served as a check on the power series results.

The nonlinear parameters, δ and ρ_0, as well as a scale factor of ρ, are chosen by the variational principle so as to minimize the energy for a given approximate eigenfunction. This choice of optimum parameters gives a great improvement in the energy for eigenfunctions containing a small number of terms. Some results obtained by us and others for the para state are given in Table I.

Table I. Energies and expectation values for the ground (para) state of $(p\text{-}\mu\text{-}p)^+$.

No. of terms in basis set	Binding energy (eV)	$\langle\rho\rangle$ [a] $(\bar{a}_\mu)$	γ_p [a] $(1/\pi)(\bar{a}_\mu)^{-3}$
	Orthogonal polynomial basis set		
8	244.8	2.895	0.5496
12	247.8	2.922	0.5704
27	249.5	2.919	0.5685
36	249.5	2.923	0.5693
64	254.0	2.969	0.5734
80	254.3	2.973	0.5733
	Power series basis set		
8	244.1	2.889	0.5472
12	247.6	2.913	0.5721
27	251.5	2.960	0.5721
36	251.5	2.968	0.5711
64	252.4		
	Results of others		
8	232.7	2.891	...[b]
1	241	...	0.654[c]
32	249	...	...[d]

[a] $\bar{a}_\mu$ is the reduced Bohr radius and is related to a_μ by $\bar{a}_\mu = a_\mu(1+M_\mu/M_p)^{-1} = 0.002847$ Å.

[b] See reference 9.

[c] See reference 1. The function $\cosh(\epsilon\rho\eta)\exp(-\frac{1}{2}f\rho\xi)$ was used, with ϵ and f chosen so as to minimize the energy.

[d] See reference 11. The basis set used was much the same as our power series basis set, but without the $-\rho^2$ term in the exponential.

Examining the convergence of the quantities in the table as the number of terms in the wave function increases suggests that the final values for the $(p\text{-}\mu\text{-}p)^+$ ground state are 254.3 eV for the binding energy[10] and $\langle\rho\rangle = 2.973\bar{a}_\mu = 0.00846$ Å ($\bar{a}_\mu$ defined in Table I) for the expectation value of the interproton separation, with error less than 1%. This value for the binding energy is 5.3 eV lower than the best previous value.[11]

Of importance in the analysis of muon capture experiments is knowledge of the muon-proton overlap, γ, which is defined as the probability per unit volume of the muon coinciding with one of the protons,[12] and is given by

$$\gamma = \frac{4}{\pi}\int_0^\infty |\Psi(\rho, 1, \pm 1)|^2 \rho^2 d\rho.$$

The overlap is expressed in units of the $(p\mu)$ atom overlap, $1/\pi\bar{a}_\mu^3$. For the para state the overlap was found to be $\gamma_p = 0.5733$, with error less than 1%. Of greater interest, however, is the muon-proton overlap for the ortho ($K = 1$) state. A 27-term, optimized-parameter wave function yielded the value $\gamma_0 = 0.500$, accurate to within a few percent error.

It should be emphasized that while the para state was treated exactly, the ortho state calculations were done with the neglect of the term H_2 in the Hamiltonian which couples the three equations defining the ortho wave function. This approximation introduces an inherent error into the wave function of the order of $(M_\mu/M_p)^2 \simeq 0.01$. A binding energy of 102.2 eV and an expectation value of the interproton separation of $\langle\rho\rangle = 3.64\bar{a}_\mu = 0.0104$ Å were calculated for the ortho state using this 27-term wave function.

It is interesting to note that the best previous computations of γ_p and γ_0 were done by Weinberg[12] using wave functions calculated by Cohen, Judd, and Riddell,[1] which had an inherent error on the order of M_μ/M_p. Weinberg's computations gave $\gamma_p = 0.654$, 14% higher than our value, and $\gamma_0 = 0.583$, 16% higher than our value. Weinberg's γ_0 was used by Rothberg et al.[4] in computing a theoretical capture rate of muons by protons in liquid hydrogen. Their theoretical capture rate was $960\gamma_0$ sec^{-1} = 560 sec^{-1} as compared to the experimental result of 464 ± 42 sec^{-1}. Using our value of γ_0 given above yields a theoretical capture rate of $960\gamma_0$ sec^{-1} = 480 sec^{-1}.

A more exact treatment of the ortho state as well as detailed discussion of these calculations will be published in the near future.

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