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ABSTRACT

An approximate method is developed for treating a generalized hydrogen-molecule ion in which two heavy particles have positive unit charges and one light particle has a negative unit charge. The expansion parameter of this approximation is the ratio of the light to the heavy mass. In first order, the method requires finding a solution to a pair of ordinary, second-order differential equations, which are coupled unless the masses of the heavy particles are equal. Explicit expressions for the coefficients in these equations are derived. The asymptotic forms of these coefficients for large nuclear separations give to first order the reduced-mass corrections to the binding energy of the light particle on either of the two heavy particles. The usual scattering theory is extended to obtain formulae for the various possible cross sections associated with this system. An iterative, variational technique for obtaining eigenvalues and eigenfunctions for bound states of the system is presented.

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I. INTRODUCTION

The experimental observation of μ^- -meson-induced fusion in a hydrogen bubble chamber¹ has led to an increased interest in the three-body system consisting of a light negatively charged particle in the presence of two heavier positively charged nuclei. This system, the generalized hydrogen molecular ion, has been treated in the past by the approximation of Born and Oppenheimer.² In this approximation the expansion parameter is the fourth root of the ratio of the mass of the light particle to that of the heavier particles. For electronic molecules this quantity is small ($\sim \frac{1}{7}$) and the approximation is sufficiently accurate to be useful in many calculations. For μ -mesonic molecules, however, the corresponding value is nearly one ($\sim \frac{2}{3}$), and the approximation is open to question.

In this paper we develop a method based on a variational approximation to the wave function of this three-body system. Although this method has the same starting point as the Born-Oppenheimer approximation--namely, the solution for the motion of the light particle with the heavy ones held fixed--it leads to an expansion parameter that is the ratio of the masses themselves. In the present approximate treatment first-order terms in this parameter have been included, while second-order ones are ignored. When the masses of the two nuclei are not equal, it is essential that the first-order terms be included, because they lead to the distinctive features of the unequal-mass case. Thus,

for example, the difference in binding energy of the light particle on one or the other of the two nuclei is contained in these terms; clearly, if the positions of the nuclei are fixed, their mass differences can play no role. In this unequal-mass case, it will be shown that the wave function of the system is obtained from the solution of a pair of coupled, ordinary, second-order differential equations in which the coupling terms come from the first-order corrections. On the other hand, if the masses of the two nuclei are equal, the pair of equations is uncoupled and the first-order terms serve only to improve the accuracy of the calculation. The development of the equations for the wave functions is given in Section II.

In Section III, the scattering states for these systems are treated. By use of the asymptotic behavior of the system of equations, explicit expressions for the elastic and exchange cross sections are derived. For unequal nuclear masses one obtains different expressions depending on whether the total energy is less than or greater than the binding energy of the light particle on the lighter nucleus. Finally, in Section IV a variational procedure for the determination of the eigenvalues and eigenfunctions of the bound states of the system is given. This method involves an iteration scheme that converges rapidly to the desired eigensolutions.

In a subsequent paper,³ the techniques that have been developed in this paper will be applied to the problem of muon-catalyzed fusion. It will be seen that close agreement with the experimental results is obtained.

II. THE THREE-BODY WAVE FUNCTION

A. The General Equations

In this section we treat the Schrödinger equation for the generalized hydrogen molecular ion consisting of two positively charged nuclei and a light negatively charged particle referred to as a meson. All particles are assumed to have unit charge.

In the development which follows, a convenient choice for a coordinate system is one in which the center-of-mass motion, the relative motion of the two nuclei, and the motion of the meson relative to the center of mass of the two nuclei are separated. If \vec{r}_1 , \vec{r}_2 , and \vec{r}_μ are the position vectors of Nucleus 1, Nucleus 2, and the meson, respectively, and m_1 , m_2 , and m_μ their masses, then the position of the center of mass, \vec{r}_c , the internucleus separation, \vec{r}_n , and the position of the meson relative to the center of mass of the two nuclei, \vec{R}_μ , are

$$\vec{r}_c = \rho_1 \vec{r}_1 + \rho_2 \vec{r}_2 + \rho_\mu \vec{r}_\mu,$$

$$\vec{r}_n = \vec{r}_1 - \vec{r}_2,$$

and

$$\vec{R}_\mu = \vec{r}_\mu - f_1 \vec{r}_1 - f_2 \vec{r}_2,$$

where

$$\rho_i = \frac{m_i}{M_t} = \frac{m_i}{m_1 + m_2 + m_\mu} \quad (\text{for } i = 1, 2, \mu)$$

and

$$f_i = \frac{m_i}{m_1 + m_2} \quad (\text{for } i = 1, 2).$$

The wave function, ψ , for the three-body system satisfies the Schrödinger equation,

$$\left[-\frac{\hbar^2}{2} \left\{ \frac{1}{M_t} \nabla_c^2 + \frac{1}{M_n} \nabla_n^2 + \frac{1}{M_\mu} \nabla_\mu^2 \right\} + V \right] \Psi = W \Psi,$$

where W is the energy and M_n and M_μ are the appropriate reduced masses, i.e.,

$$M_n = \frac{m_1 m_2}{m_1 + m_2} \quad \text{and} \quad M_\mu = \frac{m_\mu (m_1 + m_2)}{M_t}.$$

The subscripts on the Laplacians refer to derivatives with respect to the appropriate coordinates.

If all particles have unit charge, the potential V can be written as

$$V(\vec{r}_1, \vec{r}_2, \vec{r}_\mu) = \frac{e^2}{r_n} - \frac{e^2}{r_{\mu 1}} - \frac{e^2}{r_{\mu 2}} = \frac{e^2}{r_n} - \frac{e^2}{|\vec{R}_\mu - f_2 \vec{r}_n|} - \frac{e^2}{|\vec{R}_\mu + f_1 \vec{r}_n|},$$

where $r_{\mu 1}$ and $r_{\mu 2}$ are the distances between the meson and Nuclei 1 and 2 respectively; r_n is the magnitude of \vec{r}_n .

The dependence of the wave function on the center-of-mass motion is removed by the usual substitution

$$\Psi(\vec{r}_1, \vec{r}_2, \vec{r}_\mu) = e^{i\vec{P}_c \cdot \vec{r}_c / \hbar} \psi(\vec{R}_\mu, \vec{r}_n),$$

where P_c is the momentum associated with the motion of the center of mass. The resultant wave function $\psi(\vec{R}_\mu, \vec{r}_n)$ can then be expanded in terms of a complete set of functions, ψ_i , which are functions of the variable \vec{R}_μ and may contain the variable \vec{r}_n as an independent parameter. Thus we may write

$$\psi(\vec{R}_\mu, \vec{r}_n) = \sum_i \psi_i(\vec{R}_\mu, \vec{r}_n) \chi_i(\vec{r}_n) .$$

Here the functions $\chi_i(\vec{r}_n)$ are to be determined and are dependent on the choice for the $\psi_i(\vec{R}_\mu, \vec{r}_n)$.

It is convenient to choose for the ψ_i the complete set of solutions for the wave functions of the meson in the Coulomb potential of the fixed nuclei of unit charge.⁴ With such a choice the adiabatic effects of the presence of the meson on the motion of the two nuclei can be replaced by an effective potential. In this case the $\chi_i(\vec{r}_n)$ represent to lowest order the wave function describing the motion of the two nuclei.

The ψ_i are therefore the solutions to the equations

$$\mathcal{H}_\mu \psi_i(\vec{R}_\mu, \vec{r}_n) = W_i(r_n) \psi_i(\vec{R}_\mu, \vec{r}_n) ,$$

where

$$\mathcal{H}_\mu = -\frac{\hbar^2}{2M} \nabla_\mu^2 - \frac{e^2}{r_{\mu 1}} - \frac{e^2}{r_{\mu 2}} ,$$

and $W_i(r_n)$ is the energy associated with this system as a function of the parameter r_n .

If we insert the expansion for $\psi(\vec{R}_\mu, \vec{r}_n)$ into the Schrödinger equation, multiply by ψ_j , and integrate over all values of \vec{R}_μ , we obtain a set of equations

$$-\frac{\hbar^2}{2M_n} \int \psi_j(\vec{R}_\mu, \vec{r}_n) \nabla_n^2 \sum_i \chi_i(\vec{r}_n) \psi_i(\vec{R}_\mu, \vec{r}_n) d^3R_\mu + [W_j(r_n) + \frac{e^2}{r_n}] \chi_j(\vec{r}_n) = W \chi_j(\vec{r}_n) ,$$

where W is now the energy of the three-body system in its center of mass. When the indicated differentiations are carried out, the first term in this equation may be rewritten as

$$\begin{aligned}
& \int \psi_j(\vec{R}_\mu, \vec{r}_n) \sum_i \nabla_n^2 \chi_i(\vec{r}_n) \psi_i(\vec{R}_\mu, \vec{r}_n) d^3R_\mu \\
&= \nabla_n^2 \chi_j + 2 \sum_i \vec{\nabla}_n \chi_i \cdot \int \psi_j(\vec{R}_\mu, \vec{r}_n) \vec{\nabla}_n \psi_i(\vec{R}_\mu, \vec{r}_n) d^3R_\mu \\
&\quad + \sum_i \chi_i \cdot \int \psi_j(\vec{R}_\mu, \vec{r}_n) \nabla_n^2 \psi_i(\vec{R}_\mu, \vec{r}_n) d^3R_\mu .
\end{aligned}$$

Here the last term can be made more symmetric by an integration by parts:

$$\int \psi_j \nabla_n^2 \psi_i d^3R_\mu = \vec{\nabla}_n \cdot \int \psi_j \vec{\nabla}_n \psi_i d^3R_\mu - \int \vec{\nabla}_n \psi_j \cdot \vec{\nabla}_n \psi_i d^3R_\mu .$$

Finally, if we define

$$\vec{f}_{ij} = \int \psi_i \vec{\nabla}_n \psi_j d^3R_\mu = - \vec{f}_{ji}$$

and

$$g_{ij} = \int \vec{\nabla}_n \psi_i \cdot \vec{\nabla}_n \psi_j d^3R_\mu = g_{ji} ,$$

the set of Schrödinger equations becomes

$$\begin{aligned}
-\frac{\hbar^2}{2M_n} \{ \nabla_n^2 \chi_j(\vec{r}_n) + \sum_i [2\vec{f}_{ji} \cdot \vec{\nabla}_n \chi_i + (\vec{\nabla}_n \cdot \vec{f}_{ji}) \chi_i - g_{ji} \chi_i] \} \\
+ (W_j(r_n) + \frac{e^2}{r_n}) \chi_j(\vec{r}_n) = W \chi_j(\vec{r}_n) .
\end{aligned}$$

For convenience, we introduce the dimensionless parameters

$$\vec{x} = \frac{\vec{r}_n}{a_\mu} , \quad v = \frac{W}{W_\mu} ,$$

where a_μ is the Bohr radius for the mesonic atom having a reduced mesonic mass M_μ , ($a_\mu = \hbar^2 / (M_\mu e^2)$), and W_μ is the corresponding mesonic Rydberg, ($W_\mu = e^4 M_\mu / (2\hbar^2)$). All distances are measured in units of a_μ and all energies in units of W_μ . The dimensionless Schrödinger equations are then

$$-\frac{M_\mu}{M_n} \left\{ \nabla_n^2 x_j(\vec{r}_n) + \sum_i [2\vec{f}_{ji} \cdot \vec{\nabla}_n x_i + (\vec{\nabla}_n \cdot \vec{f}_{ji}) x_i - g_{ji} x_i] \right\} + (W_j(r_n) + \frac{2}{r_n}) x_j(\vec{r}_n) = W x_j(\vec{r}_n),$$

where the definitions of the symbols have been altered to refer to the dimensionless variables. We may write these equations as

$$\left\{ \nabla_n^2 + \frac{M_n}{M_\mu} [W - W_j(r_n) - \frac{2}{r_n}] \right\} x_j(\vec{r}_n) = - \sum_i \mathcal{O}_{ji} x_i(\vec{r}_n), \quad (1)$$

where

$$\mathcal{O}_{ji} = 2\vec{f}_{ji} \cdot \vec{\nabla}_n + (\vec{\nabla}_n \cdot \vec{f}_{ji}) - g_{ji}.$$

In the lowest Born-Oppenheimer approximation to the solution to these equations the dynamic correction terms \mathcal{O}_{ji} are assumed to be zero and only the x_j corresponding to the lowest W_j is retained. Furthermore, the effective potential $W_j(r_n) + 2/r_n$ is expanded about its minimum value in a power series in the displacement of r_n from its value at this minimum. While such approximations are reasonable for the treatment of the electronic molecular ions, the larger mass of meson present in the mesonic molecular ions makes these approximations less reliable.

An alternative approach, developed here includes the lowest-order dynamic corrections and makes use of exact solutions to a simplified set of Schrödinger equations. In this treatment it is necessary to separate the cases for identical and distinguishable nuclei. If the nuclei are identical, the wave functions must be either symmetric, $+$, or antisymmetric, $-$, with respect to an interchange of the two nuclei, and the two types are not coupled in the set of equations; i.e. \vec{f}_{ij} and g_{ij} are zero if i and j correspond to states of opposite symmetries. If the nuclei are not identical these terms do not vanish, and furthermore, since there is a degeneracy between the unperturbed symmetric and antisymmetric energies for large nuclear separation (corresponding to the equality of binding energy of the meson on either of the two fixed charge centers), it is necessary to include states of both symmetry in the wave function.

In our treatment we restrict ourselves to treating only the states corresponding to the lowest values of $W_i(r_n)$, designated by a zero subscript, for either of the two possible symmetries. Therefore for distinguishable (unequal-mass) nuclei our wave function is of the form

$$\psi = \psi_0^+ \chi_0^+ + \psi_0^- \chi_0^- ,$$

while for the equal-mass case

$$\text{either} \quad \psi = \psi_0^+ \chi_0^+ \quad (\text{symmetric case})$$

$$\text{or} \quad \psi = \psi_0^- \chi_0^- \quad (\text{antisymmetric case}) .$$

The errors introduced by the omission of the higher excited mesonic states cannot be accurately determined. We may, however, estimate these errors to some extent by use of a simple perturbation expansion. If we consider the

state of lowest W_i to be the dominant ones and treat $M_\mu/M_n = \epsilon$ as an expansion parameter, then for the nondegenerate (equal-mass) case we may write

$$X_0 = X_0^{(1)} + \epsilon X_0^{(2)} \dots,$$

$$X_i = \epsilon X_i^{(1)} + \epsilon^2 X_i^{(2)} \dots, \quad \text{for } i \neq 0,$$

where X_0 is the state corresponding to the lowest W_i . Inserting these expressions in the coupled equations and considering only those terms in the lowest power in ϵ , we obtain

$$X_i^{(1)} = (W - W_i - 2/r_n)^{-1} \mathcal{O}_{i0} X_0^{(1)};$$

hence, to lowest order in ϵ ,

$$X_i = (W - W_i - 2/r_n)^{-1} \epsilon \mathcal{O}_{i0} X_0.$$

If we consider the effects of the i th excited state on the equation for X_0 we note that they enter the equation only in second order in ϵ . Thus the omission of the excited states introduces errors of order ϵ^2 in the calculation of the energy of bound states. Similarly, for free states at energies such that mesonic excitations are energetically impossible even for large nuclear separations, only X_0 is necessary to determine cross sections. The errors in these cross sections are also of order ϵ^2 . In addition, for the treatment of bound states and scattering states of low energy, the denominator in the above expression is in general large due to the large separation of the excited states of the meson in the molecular ions which we shall treat.

In the degenerate (unequal-mass) case, a small perturbation can cause large changes in the wave function. It is therefore necessary to treat the two states of lowest W_1 corresponding to opposite symmetries, χ_0^+ and χ_0^- , together. The effects of the remaining higher states will, as before, introduce second-order corrections to the binding energies and cross sections.

B. The Solution for ψ_1

Although it is possible in principle to obtain exact numerical solutions to the mesonic problem with two fixed centers,⁵ the ultimate accuracy of our approximations has been shown to be limited. We therefore felt justified in using approximate variational solutions for this part of the problem.

For the symmetric solution ψ_0^+ , we assumed a variational solution of the form⁶

$$\psi_0^+ = A_+ \cosh \frac{q_+ r_n \eta}{2} e^{-\frac{p_+ r_n \xi}{2}},$$

where A_+ is the normalization constant and p_+ and q_+ are the variational parameters which minimize the expectation value of H_μ for a given value of r_n . The variables ξ and η are the usual confocal elliptic coordinates,

$$\xi = \frac{r_{\mu 1} + r_{\mu 2}}{2} \quad \text{and} \quad \eta = \frac{r_{\mu 1} - r_{\mu 2}}{2}.$$

A similar function was chosen for the antisymmetric solutions, i.e.,

$$\psi_0^- = A_- \{ \xi \} \sinh \frac{q_- r_n \eta}{2} e^{-\frac{p_- r_n \xi}{2}}.$$

Here the $\{ \xi \}$ indicates that a factor of ξ was included in the expression if this led to a lower expectation value. Specifically, for values of r_n less than r_c ($r_c \sim 1.70$) this factor was included; for values of r_n larger than

this it was omitted. For small values of r_n this additional factor is essential in order for the solution to approach the hydrogenlike 2p function as r_n approaches zero. In the neighborhood of r_c the two sets of solutions were smoothly joined.

The desired expectation values can be expressed as the sum of two terms,

$$W_i = \int \psi_i H_\mu \psi_i dt_\mu = \langle T_\mu \rangle + \langle V_\mu \rangle ,$$

where

$$\langle T_\mu \rangle = \int \psi_i T_\mu \psi_i dt_\mu = \int \vec{\nabla}_\mu \psi_i \cdot \vec{\nabla}_\mu \psi_i dt_\mu$$

and

$$\langle V_\mu \rangle = \int \psi_i V_\mu \psi_i dt_\mu = \int \psi_i \left[-2 \left(\frac{1}{r_{\mu 1}} + \frac{1}{r_{\mu 2}} \right) \right] \psi_i dt_\mu .$$

For confocal elliptic coordinates the volume element is

$$dt_\mu = \frac{r_\mu^3}{8} (\xi^2 - \eta^2) d\xi d\eta d\phi ,$$

where the limits on the variables are

$$1 \leq \xi < \infty , \quad -1 \leq \eta \leq 1 , \quad \text{and} \quad 0 \leq \phi < 2\pi .$$

The integrands in the above expressions may also be expressed in these coordinates, i.e.,

$$V_\mu = - \frac{8}{r_n} \frac{\xi}{\xi^2 - \eta^2}$$

and

$$\vec{\nabla}_\mu \psi_i \cdot \vec{\nabla}_\mu \psi_i = \frac{4}{r_n^2} \left[(\xi^2 - \eta^2) \left(\frac{d\psi_i}{d\xi} \right)^2 + (1 - \eta^2) \left(\frac{d\psi_i}{d\eta} \right)^2 \right] .$$

The integrals that occur in these and other expressions in this paper can be conveniently expressed in terms of the definite integrals

$$E_n = E_n(P) = \int_1^{\infty} e^{-P\xi} \xi^n d\xi ,$$

$$c_{2n} = c_{2n}(Q) = \int_{-1}^1 \eta^{2n} \cosh^2 \frac{Q\eta}{2} d\eta ,$$

$$c'_{2n} = c'_{2n}(Q) = \int_{-1}^1 \eta^{2n} \sinh^2 \frac{Q\eta}{2} d\eta ,$$

and

$$c_{2n+1} = c'_{2n+1} = \int_{-1}^1 \eta^{2n} \sinh \frac{Q\eta}{2} \cosh \frac{Q\eta}{2} d\eta ,$$

where $P = pr_n$ and $Q = qr_n$.

For the symmetric solution the explicit results are

$$\langle V_{\mu} \rangle_+ = -2\pi r_n^2 A_+^2 E_1 C_0 ,$$

$$\langle T_{\mu} \rangle_+ = \frac{\pi r_n A_+^2}{4} [P_+^2 (E_2 - E_0) C_0 + Q_+^2 (C'_0 - C'_2) E_0] .$$

The normalization constant A_+ is determined by the relationship

$$\frac{\pi A_+^2}{4} r_n^3 [E_2 C_0 - E_0 C_2] = 1 .$$

Similar expressions can be obtained for the antisymmetric solutions.

The minimization of the expectation values of H_{μ} for values of r_n between 0 and 20 in intervals of 0.05 were carried out with the aid of an IBM 650 digital computer. The expression for W_1 was minimized to an accuracy of eight figures; however, because of the extremal properties of W_1 , errors

due to rounding made the determination of P and Q less accurate. The results of these calculations are given graphically in Figs. 1 and 2. For comparison the results of some previous calculations of the values of W_i are included in Fig. 1. For the symmetric case with our approximate solutions we obtain $W_i = -1.20489$ for a value of r_n of 2.00. This is to be compared to the exact value of -1.20527 obtained by Hylleras.⁵ Similar agreement is found for the other values calculated by him. In view of the other approximations made in these calculations we felt that this close agreement indicated a satisfactory solution to the mesonic part of the wave function.

By making use of the analytic forms for the mesonic wave function it was possible to analytically evaluate the first-order dynamic correction terms, f_{ig} and g_{ij} , discussed in the preceding section. The specific analytic forms for these terms are given in the Appendix.

For the equal-mass case only "diagonal" correction terms occur, because the states of different symmetries are not coupled. As a consequence of the relationship $\vec{f}_{ij} = -\vec{f}_{ji}$ it follows that $f_{ii} \equiv 0$. Thus the only first-order corrections for the equal-mass case can be considered as a correction to the potential. This term is of the form

$$g_{ii} = \int \vec{\nabla}_n \psi_i \cdot \vec{\nabla}_n \psi_i dt_\mu,$$

where i denotes either + or - . This correction has been computed numerically by using the parameters obtained from the variational calculation. The results for both the symmetric and antisymmetric states in the equal-mass case are shown in Fig. 3. There has been a certain amount of controversy concerning these corrections; our results for the symmetric case are in general agreement with those of Dalgarno and McCarroll.⁷

For the unequal-mass case in which the ratio of the two masses is 1:2, similar diagonal correction terms were computed. In addition, the off-diagonal terms were obtained for this case. The results for these calculations are shown in Figs. 4 and 5.

C. Behavior for Small r_n

The study of the behavior of the mesonic solutions for small values of r_n is of considerable interest, both for the general understanding of the three-body problem and for the development of solutions to the differential equations for $X_i(r_n)$.

The behavior of the parameters p and q in this limit can be obtained by expressing the energy W_i in powers of the parameters r_n , P , and Q . For the symmetric case to lowest order in P_+ and Q_+ we have

$$-W_+ r_n^2 = -P_+^2 + 4P_+ r_n - \frac{P_+^2 Q_+^4}{240} - (P_+^2 - 4P_+ M_n) \frac{P_+^2 Q_+^2}{90} .$$

Minimizing this expression for W_+ with respect to the parameters P_+ and Q_+ , we find for

$$\begin{aligned} P_+ &\rightarrow 2r_n, & p_+ &\rightarrow 2, \\ \lim_{r_n \rightarrow 0} Q_+ &\rightarrow \frac{4}{\sqrt{3}} r_n, & q_+ &\rightarrow \frac{4}{\sqrt{3}}, \end{aligned}$$

and

$$W_+ \rightarrow -4 .$$

These results are consistent with the hydrogenlike $1s$ solution which would be expected in this limiting case. We note that the energy is relatively insensitive to the parameter q_+ in this region, occurring in terms of order r_n^4 .

In a similar manner we may obtain limiting values for the parameters p_- and q_- for the antisymmetric solution. In this case we have

$$-W_- r_n^2 = (-P_-^2 + 2r_n P_-)(1 + \frac{P_-^2 Q_-^2}{2100}) - \frac{P_-^2 Q_-^2}{2520},$$

from which it follows, for

$$\begin{aligned} P_- &\rightarrow r_n, & p_- &\rightarrow 1, \\ \lim_{r_n \rightarrow 0} Q_- &\rightarrow \sqrt{\frac{3}{5}} r_n, & q_- &\rightarrow \sqrt{\frac{3}{5}}, \end{aligned}$$

and

$$W_- \rightarrow -1,$$

which indicates that our solution ψ_- approaches a hydrogenlike 2p solution with $m_z = 0$ where the z axis is aligned in the direction of \vec{r}_n .

The asymptotic forms for g_{++} and g_{--} can be readily obtained from the complete expressions given in the Appendix. It is found that while g_{++} tends to zero in the limit of vanishing r_n , g_{--} is divergent, having a leading term of the form $2/r_n^2$. This asymptotic behavior is in fact necessary for a consistent set of solutions to the three-body system for a state in which the total angular momentum is zero. We have already seen that ψ_- approaches a p state as r_n tends to zero, hence for the total angular momentum of the system to be preserved the two nucleons must be in a relative p state. This angular dependence must be carried entirely by $\chi_-(\vec{r}_n)$, because ψ_- (or ψ_+) is a function only of the parameters r_μ , r_n and $\vec{r}_\mu \cdot \vec{r}_n$ and hence is invariant with respect to rotations of the entire system. For s states the radial wave functions, χ_- , associated with ψ_- satisfy an equation which in the

limit of small r_n is of the form

$$\frac{1}{r_n^2} \frac{d}{dr_n} \left(r_n^2 \frac{dX_-}{dr_n} \right) + \frac{2}{r_n^2} X_- + \text{terms of order } \frac{1}{r_n} = 0,$$

where the singularity in g_{--} provides the term necessary to correct the form for the X_- equation to agree with that of the usual p-state equation.

For the case in which the total angular momentum of the system is one, the situation is somewhat less clear. In this case, if the meson is in a p state it is necessary only that the nuclei be in relative s or d states. With our choice of approximate wave functions we have in fact chosen a linear combination of these states such that the potential for small r_n is $4/r_n^2$. A similar situation arises for states of higher total angular momentum, so that for small values of r_n the wave functions for antisymmetric meson states are not accurately described. For symmetric states no such ambiguities appear. This difficulty for small values of r_n is associated with the degeneracy of the various 2p states that occur for $r_n = 0$, and is therefore unimportant for larger values of r_n . To treat the inner region correctly would require the introduction of the two other 2p states and their associated X_1 's. We expect that such a treatment would, however, make small corrections to the wave functions at large distances and would be significant only for small values of r_n . For the scattering states the energies of interest to us are such that the contributions for other than s states are negligible. For the bound states, only the unequal-mass cases involve ψ_- , and the effect of this term is small except for large values of r_n . We have therefore felt justified in omitting these additional complications in our treatment.

The asymptotic behavior of \vec{f}_{+-} and g_{+-} in this limit are also of interest. From the expressions in the Appendix we obtain for

$$\lim_{r_n \rightarrow 0}, \quad \vec{f}_{+-} = 4\pi A_+ A_- (f_2 - f_1) \frac{p_+ q_-}{(p_+ + p_-)^4} \vec{e}_{r_n} = \frac{16\sqrt{2}}{81} (f_2 - f_1) \vec{e}_{r_n},$$

and for

$$\lim_{r_n \rightarrow 0}, \quad g_{+-} = -2f_{+-}/r_n,$$

where \vec{e}_{r_n} is a unit vector in the direction of r_n and $f_{+-} = \vec{f}_{+-} \cdot \vec{e}_{r_n}$.

The term g_{+-} is therefore seen to be divergent in this limit. As we shall show, the particular form of this divergence is crucial for the satisfactory solution of the differential equations.

The radial equations for a state of total angular momentum l can be obtained from Eqs. (1) by the usual substitution of ϕ_i/r_n for X_i . These equations are

$$\frac{d^2\phi_+}{dr_n^2} + \frac{1}{\epsilon} [W - V_+(r_n)] \phi_+ = -2f_{+-} \frac{d\phi_-}{dr_n} - \frac{df_{+-}}{dr_n} \phi_- + g_{+-} \phi_- \quad (2a)$$

and

$$\frac{d^2\phi_-}{dr_n^2} + \frac{1}{\epsilon} [W - V_-(r_n)] \phi_- = 2f_{+-} \frac{d\phi_+}{dr_n} + \frac{df_{+-}}{dr_n} \phi_+ + g_{+-} \phi_+, \quad (2b)$$

where

$$V_+(r_n) = W_+ + 2r_n^{-1} + \epsilon g_{++} + \epsilon l(l+1)r_n^{-2}$$

and

$$V_-(r_n) = W_- + 2r_n^{-1} + \epsilon g_{--} + \epsilon l(l+1)r_n^{-2}.$$

In order to obtain the behavior of the solutions to these equations for small values of r_n it is convenient to express the solutions in a power series in r_n ; i.e., we assume

$$\phi_+(r_n) = \sum_{t=0}^{\infty} a_t r_n^{t+K}$$

and

$$\phi_-(r_n) = \sum_{t=0}^{\infty} b_t r_n^{t+K}.$$

In addition it is necessary to expand the various other functions which appear in the equations in power series, thus

$$f_{+-} = \sum_{t=0}^{\infty} F_t r_n^t,$$

$$g_{+-} = \sum_{t=-1}^{\infty} g_t r_n^t,$$

$$V_+ = \epsilon l(l+1)r_n^{-2} + \sum_{t=-1}^{\infty} v_t r_n^t = \sum_{t=-2}^{\infty} v_t r_n^t,$$

and

$$V_- = \epsilon[l(l+1) + 2]r_n^{-2} + \sum_{t=-1}^{\infty} \mu_t r_n^t = \sum_{t=-2}^{\infty} \mu_t r_n^t.$$

Inserting these expressions into Eqs. (2a) and (2b) and equating terms with equal powers of r_n , we obtain the recursion relationships

$$\begin{aligned}
& [(t+K)(t+K-1) - \ell(\ell+1)]a_t - \frac{1}{\epsilon} \sum_{t'=0}^{t-1} v_{t'-1} a_{t-t'-1} + \frac{W}{\epsilon} a_{t-2} \\
& = \sum_{t'=0}^{t-1} [g_{t'-1} - (2t+2K-t'-2)F_{t'}] b_{t-t'-1}
\end{aligned}$$

and

$$\begin{aligned}
& [(t+K)(t+K-1) - 2 - \ell(\ell+1)]b_t - \frac{1}{\epsilon} \sum_{t'=0}^{t-1} \mu_{t'-1} b_{t-t'-1} + \frac{W}{\epsilon} b_{t-2} \\
& = \sum_{t'=0}^{t-1} [g_{t'-1} + (2t+2K-t'-2)F_{t'}] b_{t-t'-1}
\end{aligned}$$

From these equations we obtain the pair of indicial equations

$$[K(K-1) - \ell(\ell+1)] a_0 = 0$$

and

$$[K(K-1) - 2 - \ell(\ell+1)] b_0 = 0.$$

Thus if a_0 is not zero K is either $-\ell$ or $\ell+1$, while if b_0 is not zero K is equal to $\frac{1}{2} \pm [\frac{9}{4} + \ell(\ell+1)]^{1/2}$. In both these cases the solutions with the minus sign do not satisfy the conditions of integrability and may be discarded. For $\ell \neq 0$, these two cases constitute the two possible solutions to the equations. For $\ell = 0$, on the other hand, these two values for K differ by an integer, and therefore further investigation is necessary to determine whether or not two regular and independent solutions to the equations exist. It is clear that two such solutions must exist, since we must be able to describe states in which the meson is associated with either of the two nuclei

for large separations of the nuclei. If we examine the recursion equation which determines the value of b_1 in the case where $K = 1$, i.e., for $a_0 \neq 0$, we find

$$[(1 + K)K - \ell(\ell + 1) - 2]b_1 = (g_{-1} + 2b_0)a_0$$

or

$$0 \cdot b_1 = (g_{-1} + 2b_0)a_0 ;$$

this would lead to an inconsistency unless the multiplier of a_0 were zero.⁸

This is, in fact, the condition which we have shown to be true from the asymptotic behavior of the functions \vec{f}_{+-} and g_{+-} . This being true, the value of b_1 is undetermined. Thus the constant b_1 , which is arbitrary in the solution with $K = 1$, represents the fact that one can add an arbitrary amount of the solution with $K = 2$ to the solution and still retain a valid power-series expansion for small values of r_n .

D. Unitarity Current

It is of interest that one can obtain an invariant relationship between the various solutions for the system of equations describing the motion of the nuclei. If we consider two sets of solutions $\chi_{\pm}^{(1)}$ and $\chi_{\pm}^{(2)}$ to these equations, with eigenvalues W^1 and W^2 respectively, then the following equation can be constructed:

$$\int \left\{ \chi_{+}^{(2)*} \left[\left(\nabla_n^2 - \frac{1}{\epsilon} V_{+} \right) \chi_{+}^{(1)} + \theta_{+-} \chi_{-}^{(1)} \right] + \chi_{-}^{(2)*} \left[\left(\nabla_n^2 - \frac{1}{\epsilon} V_{-} \right) \chi_{-}^{(1)} + \theta_{-+} \chi_{+}^{(1)} \right] \right. \\ \left. - \chi_{+}^{(1)} \left[\left(\nabla_n^2 - \frac{1}{\epsilon} V_{+} \right) \chi_{+}^{(2)} + \theta_{+-} \chi_{-}^{(2)} \right]^* - \chi_{-}^{(1)} \left[\left(\nabla_n^2 - \frac{1}{\epsilon} V_{-} \right) \chi_{-}^{(2)} + \theta_{-+} \chi_{+}^{(2)} \right]^* \right\} d\tau_n \\ = -\frac{1}{\epsilon} \left\{ W^1 \int (\chi_{+}^{(2)*} \chi_{+}^{(1)} + \chi_{-}^{(2)*} \chi_{-}^{(1)}) d\tau_n - W^2 \int (\chi_{+}^{(1)} \chi_{+}^{(2)*} + \chi_{-}^{(1)} \chi_{-}^{(2)*}) d\tau_n \right\}$$

If W^1 is equal to W^2 then the right-hand side of the equation is zero and we find

$$\int \vec{\nabla} \cdot \vec{j}_{12} d\tau_n = 0,$$

where

$$\begin{aligned} \vec{j}_{12} = & \{ \chi_+^{(2)*} \nabla_n \chi_+^{(1)} - \chi_+^{(1)} \nabla_n \chi_+^{(2)*} + \chi_-^{(2)*} \nabla_n \chi_-^{(1)} - \chi_-^{(1)} \nabla_n \chi_-^{(2)*} \\ & + 2b_{+-} (\chi_+^{(2)*} \chi_-^{(1)} - \chi_-^{(2)*} \chi_+^{(1)}) \}. \end{aligned}$$

We shall call \vec{j}_{12} the "unitarity current". (For $\chi^{(1)} \equiv \chi^{(2)}$ this reduces to the usual expression for the probability current.) If $\chi^{(1)}$ and $\chi^{(2)}$ have the same angular dependence, then we may write

$$\begin{aligned} r_n^2 \vec{j}_{12} \cdot \vec{r}_n = r_n^2 j_{12} = & \chi_+^{(2)*} \frac{d\chi_+^{(1)}}{dr_n} - \chi_+^{(1)} \frac{d\chi_+^{(2)*}}{dr_n} \\ & - \chi_-^{(2)*} \frac{d\chi_-^{(1)}}{dr_n} - \chi_-^{(1)} \frac{d\chi_-^{(2)*}}{dr_n} \\ & + 2f_{+-} (\chi_+^{(2)*} \chi_-^{(1)} - \chi_+^{(1)} \chi_-^{(2)*}) = \text{constant}. \end{aligned}$$

Furthermore, if these solutions are regular solutions to the differential equations, their contribution to this quantity is zero because $r_n^2 j_{12}$ vanishes at the origin. Irregular solutions, on the other hand, contribute a finite amount to this expression. It follows that if $r_n^2 j_{12}$ is not zero when evaluated for any value of r_n some irregular solutions must be present.

III. SCATTERING WAVE FUNCTIONS

A. The Asymptotic Behavior for Large Values of r_n

In the limit of large values of r_n the parameters P and Q which describe the mesonic wave functions also become large. In this limit the binding energies may be expressed approximately by

$$\lim_{r_n \rightarrow \infty} -W_+ r_n^2 = -W_- r_n^2 = (P + Q - 4r_n) PQ / (P + Q) . .$$

The values of P and Q which minimize this expression for the energies are $P = Q = r_n$, for which $W_+ = W_- = -1$. This expresses qualitatively the fact that the symmetric and antisymmetric solutions for fixed nuclei can be formed from the solutions in which the meson is centered on either of the two nuclei. These eigenvalues, however, are not exactly the binding energy for such a separated system, because the units in which the eigenvalues are measured use the reduced mass for the meson with respect to the sum of the nuclear masses. The necessary corrections to the energies in this limit are contained in the asymptotic behavior of coupling terms g_{ii} . In addition, for the unequal-mass case it is necessary to obtain the splitting in the energies corresponding to the fact that the meson is more tightly bound on the heavier of the nuclei. The removal of this degeneracy in energy for this limit is contained in the off-diagonal term g_{+-} . As will be shown, both these corrections lead to expressions accurate to first order in the parameter ϵ .

The asymptotic values of g_{++} and g_{--} come entirely from the terms $I_{\xi\xi}$ and $I_{\eta\eta}$ (see Appendix) because the derivatives which occur in the remaining terms vanish in this limit. We find for

$$\lim_{r_n \rightarrow \infty}, \quad g_{++} = g_{--} = \frac{1}{2} (f_1^2 + f_2^2) \epsilon.$$

For the equal-mass case we have $f_1 = f_2 = \frac{1}{2}$, hence

$$\text{for } \lim_{r_n \rightarrow \infty}, \quad g_{++} = g_{--} = \epsilon/4,$$

and the effective potentials are corrected to give

$$\text{for } \lim_{r_n \rightarrow \infty}, \quad V_+ = V_- = -1 + \frac{1}{4} \epsilon = -1 + \frac{m}{2m_1}.$$

To first order in ϵ this is identical to M_μ^*/M_μ , where M_μ^* is the reduced mass of the meson with respect to one of the nuclei. For the unequal-mass case let us consider a system which consists of a proton (Nucleon 1), a deuteron (Nucleon 2), and a meson. In this case we have $f_1 = \frac{1}{3}$ and $f_2 = \frac{2}{3}$, and hence

$$\text{for } \lim_{r_n \rightarrow \infty}, \quad g_{++} = g_{--} = 5\epsilon/18.$$

The only term for g_{+-} which does not vanish in this limit is the term $g_{\xi\eta}$, and this leads to the result

$$\text{for } \lim_{r_n \rightarrow \infty}, \quad g_{+-} = -(f_2 - f_1)/2 = -1/6.$$

To interpret these results let us consider the asymptotic form for the radial differential equations,

$$\frac{d^2 \phi}{dr_n^2} + \frac{1}{\epsilon} (W + 1 - \frac{5}{18} \epsilon) \phi = -\frac{1}{6} \phi.$$

and

$$\frac{d^2 \phi_-}{dr_n^2} + \frac{1}{\epsilon} \left(W + 1 - \frac{5}{18} \epsilon \right) \phi_- = -\frac{1}{6} \phi_+ .$$

From these equations we obtain a new set of equations,

$$\frac{d^2 \phi_p}{dr_n^2} + \frac{1}{\epsilon} \left[W + 1 - \epsilon \left(\frac{5}{18} + \frac{1}{6} \right) \right] \phi_p = 0 \quad (3a)$$

and

$$\frac{d^2 \phi_d}{dr_n^2} + \frac{1}{\epsilon} \left[W + 1 - \epsilon \left(\frac{5}{18} - \frac{1}{6} \right) \right] \phi_d = 0 , \quad (3b)$$

where

$$\phi_p = (\phi_+ - \phi_-) / \sqrt{2} \quad \text{and} \quad \phi_d = (\phi_+ + \phi_-) / \sqrt{2} .$$

This particular choice for ϕ_p and ϕ_d is such that asymptotically ϕ_p corresponds to a total wave function in which the meson is centered on Nucleon 1, while ϕ_d is the corresponding case for Nucleon 2. The binding energy of the meson is that value of W for which the kinetic energy of the relative nuclear motion is zero ($\frac{d^2 \phi}{dr_n^2} = 0$). Thus we find, for the binding energies,

$$W_p = -1 + \frac{4\epsilon}{9}$$

and

$$W_d = -1 + \frac{\epsilon}{9} .$$

These expressions are the correct binding energies to first order in the parameter ϵ .

B. Scattering Cross Sections

In the treatment which follows we restrict ourselves to the consideration of the scattering states of zero total angular momentum; the extension to states of higher angular momentum, however, is straightforward. For the investigation of scattering phenomena, as in the usual treatments, we need study only the asymptotic behavior of the wave functions for the separated system.

For the unequal-mass case there are four asymptotic functions to consider, i.e., χ_+ and χ_- for each of the two solutions regular at the origin. In addition, as we have shown in the preceding section, the degeneracy of the binding energies of the meson on the two separated nuclei has been removed by the dynamic correction terms. It is therefore necessary to distinguish between the case in which the energy of the system lies between these two binding energies and the case in which it is larger than either of them. These two energy ranges correspond to different physical situations. In the former the only scattering states allowed are those in which the meson is bound to the heavier nucleus for large separations. In the latter the meson may be bound to either of the nuclei; exchange processes are also possible in this case.

It is once again convenient to use wave functions that asymptotically describe the meson centered on one of the two nuclei. We therefore define

$$\phi_p^i = (\phi_+^i - \phi_-^i) / \sqrt{2},$$

and

$$\phi_d^i = (\phi_+^i + \phi_-^i) / \sqrt{2}.$$

Here ϕ_p is the radial wave function whose form corresponds to the meson bound on Nucleus 1, the lighter nucleus, with an energy W_p ; ϕ_d and W_d are defined in a similar manner for the heavier nucleus. (If we consider the

system of a proton, a deuteron, and a meson, the expressions of the preceding section define W_p and W_d .) The superscripts i ($i = 1, 2$) refer to either of the two regular solutions to the radial differential equations.

If the energy, W , is such that $W_d \leq W \leq W_p$, then we can write the asymptotic behavior for ϕ_p and ϕ_d in the form

$$\phi_p = a_p^i e^{\alpha r_n} + b_p^i e^{-\alpha r_n}$$

and

$$\phi_d = a_d^i \sin(k_d r_n + \delta_d^i),$$

where $\alpha = [(W_p - W)/\epsilon]^{1/2}$ and $k_d = [(W - W_d)/\epsilon]^{1/2}$. The parameters

a_p^i , b_p^i , a_d^i , and δ_d^i are determined by the value of ϕ_p^i , $d\phi_p^i/dr_n$, ϕ_d^i , and $d\phi_d^i/dr_n$ evaluated for some large value of r_n . In order to completely specify the wave function it is necessary to determine that linear combination of the two solutions $i = 1$ and $i = 2$ for which no increasing exponential remains in the asymptotic expression for ϕ_p . We may also normalize these solutions to the incident part of the plane wave. If this is done we find, for the corresponding wave functions χ_p and χ_d in this asymptotic limit, the forms¹⁰

$$\chi_p \propto \frac{e^{-\alpha r_n}}{r_n}$$

and

$$\chi_d = e^{ik_d z} + \left(\frac{M-1}{2ik_d} \right) \frac{e^{ik_d r_n}}{r_n},$$

where the z axis is in the direction of the incident-particle beam. The quantity M is defined as

$$M = \frac{a_p^1 a_d^2 e^{i\delta_d^2} - a_p^2 a_d^1 e^{i\delta_d^1}}{a_p^1 a_d^2 e^{-i\delta_d^2} - a_p^2 a_d^1 e^{-i\delta_d^1}}$$

If we replace M by the quantity $e^{2i\theta_d}$, then θ_d may be considered the phase shift for this scattering, and the scattering cross section can be written in the usual form,

$$\sigma = \frac{4\pi}{k_d^2} \sin^2 \theta_d .$$

If the energy is larger than W_p , then both solutions have asymptotic sinusoidal behavior, i.e.,

$$\phi_p^i = a_p^i \sin(k_p r_n + \delta_p^i)$$

and

$$\phi_d^i = a_d^i \sin(k_d r_n + \delta_d^i) ,$$

where $k_p = [(W - W_p)/\epsilon]^{1/2}$. There are now two possible physical states corresponding to incident states in which the meson is centered on either of the two nuclei. In this case, however, we may separately choose those linear combinations of the two sets of solutions that correspond to no incident part for either the χ_p or the χ_d . In either case we may normalize the solutions to the incident wave.

For the scattering of the p-mesonic system from a d nucleus, we obtain the asymptotic forms

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$$\chi_p = e^{ik_p z} + h_{pp} e^{ik_p r_n / r_n},$$

$$\chi_d = h_{pd} e^{ik_d r_n / r_n},$$

where

$$h_{pp} = [(a_p^2 a_d^1 e^{i(\delta_p^2 - \delta_d^1)} - a_p^1 a_d^2 e^{i(\delta_p^1 - \delta_d^2)}) D^{-1} - 1] / 2ik_p,$$

$$h_{pd} = a_d^1 a_d^2 \sin(\delta_d^1 - \delta_d^2) / Dk_p,$$

and

$$D = a_p^2 a_d^1 e^{-i(\delta_p^2 + \delta_d^1)} - a_p^1 a_d^2 e^{-i(\delta_p^1 + \delta_d^2)}.$$

Here h_{pp} gives the amplitude for normal scattering and h_{pd} the corresponding amplitude for exchange scattering in which the meson is captured by the heavier nucleus. The cross sections for these cases are

$$\sigma_{pp} = 4\pi |h_{pp}|^2,$$

and for the exchange process,

$$\sigma_{pd} = 4\pi |h_{pd}|^2 / k_d k_p,$$

where the factor k_d/k_p is necessary to correct for the change in velocity of the incident and outgoing particles in this inelastic collision.

In a similar fashion the scattering of the d-mesonic system from a p nucleus can be obtained. In this case we find

$$h_{dd} = [(a_p^2 a_d^1 e^{i(\delta_d^1 - \delta_p^2)} - a_p^1 a_d^2 e^{i(\delta_d^2 - \delta_p^1)}) D^{-1} - 1] / 2ik_d$$

and

$$h_{dp} = a_p^1 a_p^2 \sin(\delta_p^1 - \delta_p^2) / Dk_d .$$

The corresponding cross sections are

$$\sigma_{dd} = 4\pi |h_{dd}|^2$$

and

$$\sigma_{dp} = 4\pi |h_{dp}|^2 k_p/k_d .$$

From the conservation of unitarity current one can show $h_{pd} = h_{dp}$ and that the two exchange cross sections are simply related.

For the equal-mass case the phase shifts for the symmetric and antisymmetric scattering states may be independently evaluated by use of the asymptotic forms

$$\chi_i = a_i \sin(kr_n + \delta_i) / r_n , \quad (\text{for } i = +, -) ,$$

where $k = [(W - 1 + \epsilon/4)/\epsilon]^{1/2}$. In this case, however, a further complication is introduced because the nuclei are generally identical particles. In such cases the total wave functions for the system must be properly symmetrized. As before, it is convenient to introduce combinations of wave functions which describe the states corresponding to the meson centered on each of the two nuclei for large separations. For the case in which the meson is centered on Nucleus 1 the mesonic wave function is

$$\psi_1 = (\psi_+ - \psi_-) / \sqrt{2} ,$$

with a corresponding nucleonic wave function,

$$x_1 = (x_+ - x_-) / \sqrt{2} .$$

The wave functions for the other case are

$$\psi_2 = (\psi_+ + \psi_-) / \sqrt{2}$$

and

$$x_2 = (x_+ + x_-) / \sqrt{2} .$$

The total wave function is then of the form

$$\bar{\Psi} = x_1 \psi_1 + x_2 \psi_2 .$$

Before symmetrization, the solution which corresponds to an incident system in which the meson is associated with Nucleus 1 or with Nucleus 2 has the asymptotic forms

$$\left\{ \begin{array}{l} x_1 = e^{ikz} + h_{11} r_n^{-1} e^{ikr_n} \\ x_2 = h_{12} r_n^{-1} e^{ikr_n} \end{array} \right.$$

and

$$\left\{ \begin{array}{l} x_1 = h_{21} r_n^{-1} e^{ikr_n} \\ x_2 = e^{-ikz} + h_{22} r_n^{-1} e^{ikr_n} \end{array} \right.$$

respectively. Using the asymptotic forms for x_+ and x_- , we find

$$h_{11} = h_{22} = (4ik)^{-1} [e^{2i\delta_+} + e^{2i\delta_-} - 2]$$

and

$$h_{12} = h_{21} = (4ik)^{-1} [e^{2i\delta_+} - e^{-2i\delta_-}] .$$

For a system consisting of a meson and two spin- $\frac{1}{2}$ particles such as protons, the total wave function must be symmetric for singlet states (s) and antisymmetric for triplet states (t). Thus for states of zero total angular momentum the total wave functions are¹⁰

$$\Psi_{s,t} = e^{ikz} \psi_1 \pm e^{-ikz} \psi_2 + (h_{11} \pm h_{12})(e^{ikr_n}/r_n) (\psi_1 \pm \psi_2) .$$

From this wave function we obtain for the cross sections¹¹

$$\sigma_{\text{singlet}} = 4\pi | h_{11} + h_{12} |^2 = 4\pi k^{-2} \sin^2 \delta_+ ,$$

$$\sigma_{\text{triplet}} = 4\pi | h_{11} - h_{12} |^2 = 4\pi k^{-2} \sin^2 \delta_- .$$

The total cross section is

$$\sigma_{pp} = 4\pi k^{-2} [\frac{1}{4} \sin^2 \delta_+ + \frac{3}{4} \sin^2 \delta_-] .$$

Similarly we find, for the case in which the two nuclei are deuterons,

$$\sigma_{dd} = 4\pi k^{-2} [\frac{2}{3} \sin^2 \delta_+ + \frac{1}{2} \sin^2 \delta_-] .$$

IV. BOUND STATES

This section is devoted to a discussion of an iterative scheme by which it is possible to obtain the bound-state eigenvalues and eigenfunctions for the system of differential equations describing the nuclear motion. In this development it is assumed that the integration of the differential equations can be carried out by either exact or numerical methods.

For the unequal-mass case, the Hamiltonian for the nuclear system can be written as

$$H = \int_0^{\infty} \left\{ \left(\frac{d\phi_+}{dr_n} \right)^2 + \left(\frac{d\phi_-}{dr_n} \right)^2 + \frac{V_+}{\epsilon} \phi_+^2 + \frac{V_-}{\epsilon} \phi_-^2 + \frac{l(l+1)}{r_n^2} (\phi_+^2 + \phi_-^2) - 2g_{+-} \phi_+ \phi_- + 2f_{+-} \left(\phi_+ \frac{d\phi_-}{dr_n} - \phi_- \frac{d\phi_+}{dr_n} \right) \right\} dr_n.$$

If we consider variations of ϕ_+ , where ϕ_+ is assumed to be continuous with a piecewise continuous first derivative, subject to the constraint that

$$\int_0^{\infty} (\phi_+^2 + \phi_-^2) dr_n = 1, \text{ then the variation of } H \text{ is}$$

$$\delta H = \int_0^{\infty} 2 \left\{ -\frac{d^2\phi}{dr_n^2} + \left(\frac{V_+}{\epsilon} + \frac{l(l+1)}{r_n^2} \right) \phi_+ - g_{+-} \phi_- + 2f_{+-} \frac{d\phi_-}{dr_n} + \phi_- \frac{df_{+-}}{dr_n} \right\} \delta \phi_+ dr_n + \lambda \int_0^{\infty} 2\phi_+ \delta \phi_+ dr_n + \sum_i \delta \phi_+(r_i) \Delta_i \left(\frac{d\phi_+}{dr_n} \right).$$

Here r_i indicates the values of r_n at the points of discontinuity, of $d\phi_+/dr_n$, and $\Delta_i \left(\frac{d\phi_+}{dr_n} \right)$ are the changes in $d\phi_+/dr_n$ between $r_i - |\nu|$ and $r_i + |\nu|$ in the limit of vanishing ν . If the parameter λ is $-W/\epsilon$,

then the conditions for an extremum in H are that the radial differential equation for ϕ_+ be satisfied and $d\phi_+/dr_n$ be continuous. In a similar manner the variations of H with respect to variations of ϕ_- lead to the radial equations for ϕ_- . The value of H obtained for this extremum is in fact W/ϵ .

If we now use trial wave functions $\phi_+^{(0)}$ and $\phi_-^{(0)}$ that (a) satisfy the differential equations for an energy W^0 , (b) are continuous for all values of r_n , and (c) have continuous first derivatives except at one point r_0 , then the true eigenvalue W^T may be expressed as

$$\begin{aligned}
 W^T \int_0^\infty (\phi_+^{(0)2} + \phi_-^{(0)2}) dr_n &= \int_0^\infty \phi_+^{(0)} \left\{ -\frac{d^2\phi_+^{(0)}}{dr_n^2} + \frac{V_+}{\epsilon} \phi_+^{(0)} \right. \\
 &+ \left. \frac{\ell(\ell+1)}{r_n^2} \phi_n^{(0)} - g_{+-} \phi_-^{(0)} + 2f_{+-} \frac{d\phi_-^{(0)}}{dr_n} + \phi_-^{(0)} \frac{df_{+-}}{dr_n} \right\} dr_n \\
 &+ \int_0^\infty \phi_-^{(0)} \left\{ -\frac{d^2\phi_-^{(0)}}{dr_n^2} + \frac{V_-}{\epsilon} \phi_-^{(0)} + \frac{\ell(\ell+1)}{r_n^2} \phi_-^{(0)} - g_{+-} \phi_+^{(0)} \right. \\
 &\quad \left. - 2f_{+-} \frac{d\phi_+^{(0)}}{dr_n} - \phi_+^{(0)} \frac{df_{+-}}{dr_n} \right\} dr_n \\
 &- \left\{ \phi_+^{(0)}(r_0) \Delta_0 \left(\frac{d\phi_+^{(0)}}{dr_n} \right) + \phi_-^{(0)}(r_0) \Delta_0 \left(\frac{d\phi_-^{(0)}}{dr_n} \right) \right\} .
 \end{aligned}$$

As a result of condition (a) and the extremal nature of H for this solution, this may be rewritten as

$$W^T = W^0 - \frac{\left\{ \phi_+^{(0)}(r_0) \Delta_0 \left(\frac{d\phi_+^{(0)}}{dr_n} \right) + \phi_-^{(0)}(r_0) \Delta_0 \left(\frac{d\phi_-^{(0)}}{dr_n} \right) \right\}}{\int_0^\infty \left\{ \phi_+^{(0)2} + \phi_-^{(0)2} \right\} dr_n} + o(\xi^2),$$

where ξ is a parameter of smallness that indicates the deviation between the trial and true solutions.

The integration for the bound states can be divided into two regions, with r_m as the common boundary. At this point four independent quantities can be specified, namely, $\phi_+^{(0)}$, $d\phi_+^{(0)}/dr_n$, $\phi_-^{(0)}$, and $d\phi_-^{(0)}/dr_n$. By choosing appropriate linear combinations of the two regular inner solutions and the two bounded outer solutions, three of the four quantities can be made continuous at r_m .¹² For the correct eigenvalue the fourth quantity will also be continuous. For a trial eigenvalue in general one of the four quantities will not be continuous, however. If, for example, we allow this discontinuity to occur in $d\phi_+^{(0)}/dr_n$, then a better approximation to the correct eigenvalue, W^n , is expressed in terms of the trial eigenvalue and the value of the function at r_m as

$$W^n = W^0 + \frac{\phi_+^{(0)} \left[\left(\frac{d\phi_+^{(0)}}{dr_n} \right)_{r=|\gamma|} - \left(\frac{d\phi_+^{(0)}}{dr_n} \right)_{r=|\gamma|} \right]}{\int \phi_+^{(0)2} + \phi_-^{(0)2} dr_n}.$$

By using this new improved eigenvalue to obtain a new trial solution and thus iterate the solution, we can converge upon the correct eigenvalue and consequently the correct eigenfunction.

This variational procedure is not restricted to the ground state, but may be applied to the higher excited states as well. The determination of a specific state merely requires the specification of a boundary condition on the number of nodes allowed in the solution.

For the equal-mass case the development given above is equally applicable. In this case the ϕ_+ and ϕ_- equations are not coupled. Bound states, however, occur only for the ϕ_+ solutions. It therefore suffices to impose on the development given above the added constraint $\phi_- \equiv 0$.

APPENDIX

In this appendix we obtain explicit analytic expressions for the first-order dynamic corrections for the case in which the mesonic wave functions are assumed to be those used in the text, i.e.,

$$\psi_+ = A_+ \cosh \frac{q_+ r_n \eta}{2} e^{-\frac{p_+ r_n \xi}{2}}$$

and

$$\psi_- = A_- (\xi) \sinh \frac{q_- r_n \eta}{2} e^{-\frac{p_- r_n \xi}{2}}$$

The dynamic correction terms are of the form

$$g_{ij} = g_{ji} = \int \vec{\nabla}_n \psi_i \cdot \vec{\nabla}_n \psi_j d\tau_\mu$$

and

$$\vec{f}_{ij} = -\vec{f}_{ji} = \int \psi_i \vec{\nabla}_n \psi_j d\tau_\mu,$$

where, from the previous development, the indicated differentiations, $\vec{\nabla}_n$, must be carried out with the mesonic variable \vec{R}_μ fixed.

For the symmetric case, we may write

$$\frac{\vec{\nabla}_n \psi_+}{\psi_+} = \vec{e}_{r_n} \left\{ \frac{1}{A_+} \frac{dA_+}{dr_n} + \frac{r_n \eta}{2} \frac{dq_+}{dr_n} \tanh \frac{q_+ r_n \eta}{2} - \frac{r_n \xi}{2} \frac{dp_+}{dr_n} \right\} \\ + \frac{q_+}{2} \vec{\nabla}_n(r_n \eta) \tanh \frac{q_+ r_n \eta}{2} - \frac{p_+}{2} \vec{\nabla}_n(r_n \xi),$$

where \vec{e}_{r_n} is a unit vector in the direction of \vec{r}_n . For reference we designate these five terms by the subscripts A, q, p, η , and ξ , respectively.

Similarly for the antisymmetric cases for $r_n > r_c$, we have

$$\frac{\vec{\nabla}_n \psi_-}{\psi_-} = \vec{e}_{r_n} \left\{ \frac{1}{A_-} \frac{dA_-}{dr_n} + \frac{r_n \eta}{2} \frac{dq_-}{dr_n} \coth \frac{q_- r_n \eta}{2} - \frac{r_n \xi}{2} \frac{dp_-}{dr_n} \right\} \\ + \frac{q_-}{2} \vec{\nabla}_n(r_n \eta) \coth \frac{q_- r_n \eta}{2} - \frac{p_-}{2} \vec{\nabla}_n(r_n \xi) ,$$

while for $r_n < r_c$, we write

$$\frac{\vec{\nabla}_n \psi_-}{\psi_-} = \vec{e}_{r_n} \left\{ \left(\frac{1}{A_-} \frac{dA_-}{dr_n} - \frac{1}{r_n} \right) + \frac{r_n \eta}{2} \frac{dq_-}{dr_n} \coth \frac{q_- r_n \eta}{2} - \frac{r_n \xi}{2} \frac{dp_-}{dr_n} \right\} \\ + \frac{q_-}{2} \vec{\nabla}_n(r_n \eta) \coth \frac{q_- r_n \eta}{2} - \left(\frac{p_-}{2} - \frac{1}{r_n \xi} \right) \vec{\nabla}_n(r_n \xi) .$$

In order to obtain the expressions for g_{ij} and f_{ij} the following identities are useful:

$$\vec{\nabla}_n(r_n \xi) \cdot \vec{\nabla}_n(r_n \xi) = f_1^2 + f_2^2 - 2f_1 f_2 \frac{\xi^2 + \eta^2 - 2}{\xi^2 - \eta^2} ,$$

$$\vec{\nabla}_n(r_n \eta) \cdot \vec{\nabla}_n(r_n \eta) = f_1^2 + f_2^2 + 2f_1 f_2 \frac{\xi^2 + \eta^2 - 2}{\xi^2 - \eta^2} ,$$

$$\vec{\nabla}_n(r_n \xi) \cdot \vec{\nabla}_n(r_n \eta) = f_2 - f_1 ,$$

$$\vec{\nabla}_n(r_n \xi) \cdot \vec{e}_{r_n} = \frac{1}{\xi^2 - \eta^2} \{ \xi(1 - \eta^2) + (f_2 - f_1)\eta(\xi^2 - 1) \} ,$$

$$\vec{\nabla}_n(r_n \eta) \cdot \vec{e}_{r_n} = \frac{1}{\xi^2 - \eta^2} \{ (f_2 - f_1)\xi(1 - \eta^2) + \eta(\xi^2 - 1) \} .$$

Using the above expressions, we may evaluate each of the terms that occur.

For g_{++} we obtain the sum of the following terms:

$$I_{A,A}^+ = \left(\frac{1}{A_+} \frac{dA_+}{dr_n} \right)^2 ,$$

$$I_{p,p}^+ = N \frac{r_n^2}{4} \left(\frac{dp_+}{dr_n} \right)^2 (E_4 C_0 - E_2 C_2) ,$$

$$I_{q,q}^+ = N \frac{r_n^2}{4} \left(\frac{dq_+}{dr_n} \right)^2 (E_2 C'_2 - E_0 C'_4) ,$$

$$I_{pq}^+ = -N \frac{r_n^2}{2} \left(\frac{dp_+}{dr_n} \right) \left(\frac{dq_+}{dr_n} \right) (E_3 C_1 - E_1 C_3) ,$$

$$I_{p,A}^+ = -N \left(\frac{1}{A_+} \frac{dA_+}{dr_n} \right) r_n \left(\frac{dp_+}{dr_n} \right) (E_3 C_0 - E_1 C_2) ,$$

$$I_{q,A}^+ = N \left(\frac{1}{A_+} \frac{dA_+}{dr_n} \right) r_n \left(\frac{dq_+}{dr_n} \right) (E_2 C_1 - E_0 C_3) ,$$

$$I_{\eta,\eta}^+ = N \frac{q_+^2}{4} \{ (f_1^2 + f_2^2) [E_2 C'_0 - E_0 C'_2] + 2f_1 f_2 [E_2 C'_0 + E_0 C'_2 - 2E_0 C'_0] \} ,$$

$$I_{\xi,\eta}^+ = 0 ,$$

$$I_{\eta,p}^+ = -N r_n q_+ C_1 \frac{(E_3 - E_1)}{2} ,$$

$$I_{\eta,q}^+ = N r_n q_+ C'_2 \frac{(E_2 - E_0)}{2} ,$$

$$I_{\xi, A}^+ = -N \left(\frac{1}{A_+} \frac{dA_+}{dr_n} \right) p_+ E_1 (C_0 - C_2) ,$$

$$I_{\eta, A}^+ = N \left(\frac{1}{A_+} \frac{dA_+}{dr_n} \right) q_+ C_1 (E_2 - E_0) ,$$

$$I_{\xi, \xi}^+ = \frac{p_+^2}{4} \{ r_1^2 + r_2^2 - 2r_1 r_2 N [E_2 C_0 + E_0 C_2 - 2E_0 C_0] \} ,$$

$$I_{\xi, q}^+ = -N r_n p_+ E_1 \frac{(C_1 - C_2)}{2} ,$$

$$I_{\xi, p}^+ = N r_n p_+ E_2 \frac{(C_0 - C_2)}{2} ,$$

where $N = (E_2 C_0 - E_0 C_2)^{-1}$. The subscripts indicate the pairs of terms involved.

A similar set of terms is obtained for g_{--} . For $r_n > r_0$ these differ from the above not only in that p_+ and q_+ are replaced by p_- and q_- , but also by the interchange of C_{2n} and C'_{2n} . For $r_n < r_0$ several additional changes occur:

(a) $\frac{1}{A_+} \frac{dA_+}{dr_n}$ is replaced by $\left(\frac{1}{A_+} \frac{dA_+}{dr_n} - \frac{1}{r_n} \right)$,

(b) E_n is replaced by E_{n+2} ,

(c) in the last two terms $p_+ E_n$ is replaced by $p_- E_{n+2} - \frac{2}{r_n} E_{n+1}$,
and

(d) $I_{\xi, \xi}^-$ has the form

$$\begin{aligned}
I_{\xi, \xi}^- &= \frac{p_-^2}{4} \{ f_1^2 + f_2^2 - 2f_1 f_2 N [E_4 C'_0 + E_2 C'_2 - 2E_2 C'_0] \} \\
&+ \frac{p}{2r_n} f_1 f_2 N [E_3 C'_0 + E_1 C'_2 - 2E_1 C'_0] \\
&- \frac{1}{r_n^2} f_1 f_2 N [E_2 C'_0 + E_0 C'_2 - 2E_0 C'_0] .
\end{aligned}$$

In the calculation for f_{+-} , only those terms containing either $\vec{\nabla}_n(r_n \xi)$ or $\vec{\nabla}_n(r_n \eta)$ give a result different from zero because the others lead to integrands odd in the variable η . Thus we find

$$\begin{aligned}
f_{+-} &= \frac{\pi r_n^3}{16} A_+ A_- (f_2 - f_1) \{ p_+ (E_2 - E_0) [C_1(\xi) + C_1(\Delta)] \\
&- q_+ E_1 [C_0(\xi) - C_0(\Delta) - C_2(\xi) + C_2(\Delta)] \} ,
\end{aligned}$$

where $\Sigma p = p_+ + p_-$, $\Sigma = (q_+ + q_-)/2$, and $\Delta = (q_+ - q_-)/2$. The argument of the terms E_n is (Σp) . This expression is valid for $r \geq r_c$; for $r < r_c$, E_n becomes E_{n+1} .

Finally we obtain the expression for g_{+-} as $(f_2 - f_1) A_+ A_- \frac{\pi r_n^3}{4}$ times the sum of the terms

$$g_{\xi, \eta} = - \frac{p_+ q_-}{4} \{ E_2 [C_0(\Sigma) + C_0(\Delta)] - E_0 [C_2(\Sigma) + C_2(\Delta)] \} ,$$

$$g_{\eta, \xi} = - \frac{q_+ p_-}{4} \{ E_2 [C_0(\Sigma) - C_0(\Delta)] - E_0 [C_2(\Sigma) - C_2(\Delta)] \} ,$$

$$\xi_{A,\xi} = -\frac{1}{A_+} \frac{dA_+}{dr_n} \frac{p_-}{2} (E_2 - E_0) [C_1(\Sigma) - C_1(\Delta)] ,$$

$$\xi_{\xi,A} = -\frac{1}{A_-} \frac{dA_-}{dr_n} \frac{p_+}{2} (E_2 - E_0) [C_1(\Sigma) - C_1(\Delta)] ,$$

$$\xi_{p,\xi} = +\frac{r_n p_-}{4} \frac{dp_+}{dr_n} (E_3 - E_1) [C_1(\Sigma) - C_1(\Delta)] ,$$

$$\xi_{\xi,p} = \frac{r_n p_+}{4} \frac{dp_-}{dr_n} (E_3 - E_1) [C_1(\Sigma) - C_1(\Delta)] ,$$

$$\xi_{q,\xi} = -\frac{r_n p_-}{4} \frac{dq_+}{dr_n} (E_2 - E_0) [C_2(\Sigma) - C_2(\Delta)] ,$$

$$\xi_{\xi,q} = -\frac{r_n p_+}{4} \frac{dq_-}{dr_n} (E_2 - E_0) [C_2(\Sigma) + C_2(\Delta)] ,$$

$$\xi_{A,\eta} = \frac{1}{A_+} \frac{dA_+}{dr_n} \frac{q_-}{2} E_1 [C_0(\Sigma) + C_0(\Delta) - C_2(\Sigma) - C_2(\Delta)] ,$$

$$\xi_{\eta,A} = \frac{1}{A_-} \frac{dA_-}{dr_n} \frac{q_+}{2} E_1 [C_0(\Sigma) - C_0(\Delta) - C_2(\Sigma) + C_2(\Delta)] ,$$

$$\xi_{p,\eta} = -\frac{r_n q_-}{4} \frac{dp_+}{dr_n} E_1 [C_0(\Sigma) + C_0(\Delta) - C_2(\Sigma) - C_2(\Delta)] ,$$

$$\xi_{\eta,p} = -\frac{r_n q_+}{4} \frac{dp_-}{dr_n} E_2 [C_0(\Sigma) - C_0(\Delta) - C_2(\Sigma) + C_2(\Delta)] ,$$

$$\xi_{q,\eta} = \frac{r_n q_-}{4} \frac{dq_+}{dr_n} E_1 [C_1(\Sigma) + C_1(\Delta) - C_3(\Sigma) - C_3(\Delta)] ,$$

$$\xi_{\eta,q} = \frac{r_n q_+}{4} \frac{dq_-}{dr_n} E_1 [C_1(\Sigma) + C_1(\Delta) - C_3(\Sigma) - C_3(\Delta)] .$$

Again, for $r < r_c$, modifications such as have already been pointed out must be made: $\frac{1}{A_-} \frac{dA_-}{dr_n}$ is replaced by $\frac{1}{A_-} \frac{dA_-}{dr_n} - \frac{1}{r_n}$, E_n by E_{n+1} , and $p_- E_n$ by $p_- E_{n+1} - \frac{2}{r_n} E_n$ in these expressions.

FOOTNOTES

1. Alvarez, Bradner, Crawford, Falk-Vairant, Good, Gow, Rosenfeld, Solmitz, Stevenson, Ticho, and Tripp, Phys. Rev. 105, 1127 (1957).
2. M. Born and J. R. Oppenheimer, Z. Physik 46, 814 (1928); Z. Physik 50, 347 (1928).
3. Cohen, Judd, and Riddell, Mu-Mesonic Molecules: II. Molecular-Ion Formation and Nuclear Catalysis, UCRL-8391, May 1959.
4. The ground state and some of the excited states for this system have been studied, e.g., by E. A. Hylleras, Z. Physik 71, 739 (1931); Edward Teller, Z. Physik 61, 458 (1930); and Bates, Ledsham, and Stewart, Phil. Trans. Roy. Soc. London, Ser. A, 246, 215 (1953-4).
5. E. A. Hylleras, loc. cit.
6. This form was used in treating the hydrogen molecular ion by V. Guillemin, Jr. and C. Zener, Proc. Natl. Acad. Sci. U.S. 15, 314 (1929).
7. A. Dalgarno and R. McCarroll, Proc. Roy. Soc. (London) A237, 383 (1956). The results of T. Y. Wu, J. Chem. Phys. 24, 444 (1956) and T. Y. Wu and A. B. Bhatia, J. Chem. Phys. 24, 48 (1956) are in disagreement with ours.
8. If such a conflict exists, the second solution will be of a logarithmic type.
9. By generalizing the functions ψ_+ and ψ_- to the form $\psi = \alpha \psi_+ + \beta \psi_-$ and including in the Hamiltonian those terms in g_{++} , g_{--} , and g_{+-} that are independent of derivatives of p , q , etc., one could obtain the exact binding energy as $r_n \rightarrow \infty$, without changing the form of the differential equation for the X 's. Because physical processes would still involve unknown terms of order ϵ^2 , it was felt that the additional labor involved in such a treatment was not justified.

10. It might be pointed out that this asymptotic form has a defect in that the meson current is zero. This is consistent with the assumption that the meson velocity about the nuclei is large compared with the nuclear velocities, and therefore, in the region where the particles interact strongly, such additional velocities represent a small correction. A correct asymptotic form for the plane-wave part would be

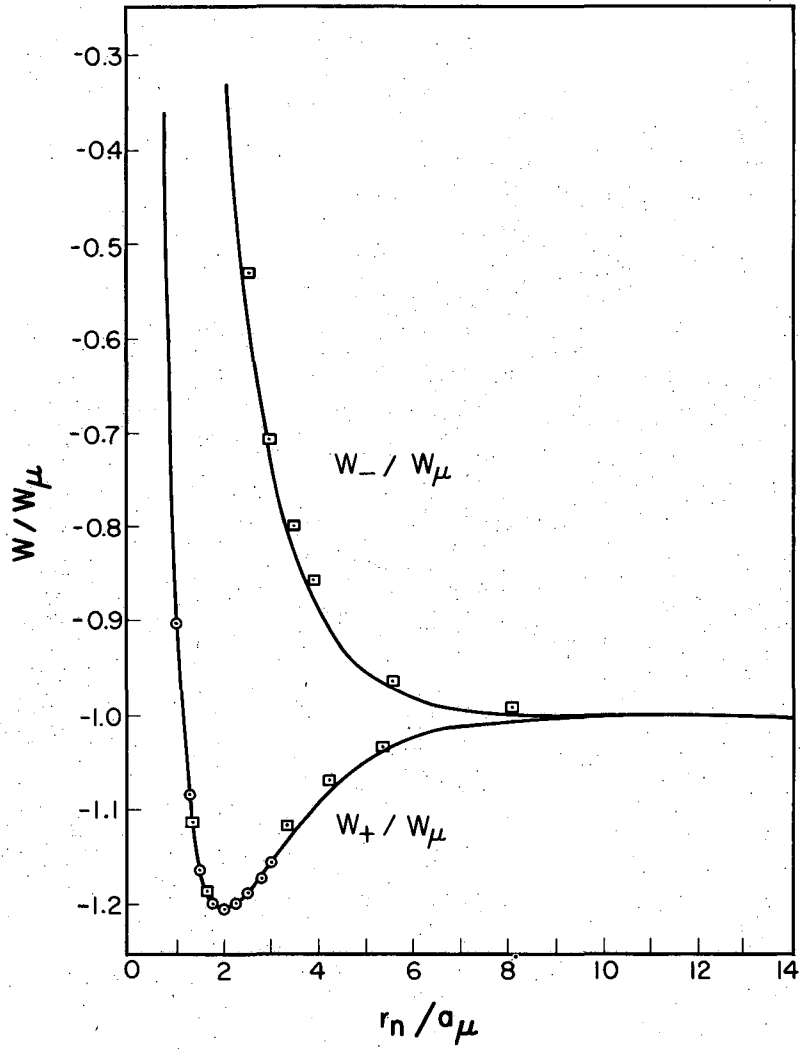
$$e^{i[kz_{\mu} + k'z_1 - (k + k')z_2]} f(\vec{r}_{\mu} - \vec{r}_1) ,$$

where $k/m_1 = k'/m_{\mu}$ and f is the wave function for the meson about Nucleus 1. Our wave function thus neglects $k' = (m_{\mu}/m_1)k$.

11. It is perhaps of interest that this result is the same as that which would have been obtained for nonidentical particles. The presence of the meson on one of the two particles provides some basis for distinguishing between them. The result follows directly from second quantization of the system.
12. If, as was done for the bound states, the integration is divided into two regions for free states with $W_D \leq W < W_P$, three bounded outer solutions exist (two sinusoidal ones associated with ψ_D and a decreasing-exponential one associated with ψ_H). This gives the necessary freedom to make all four quantities continuous at r_m .

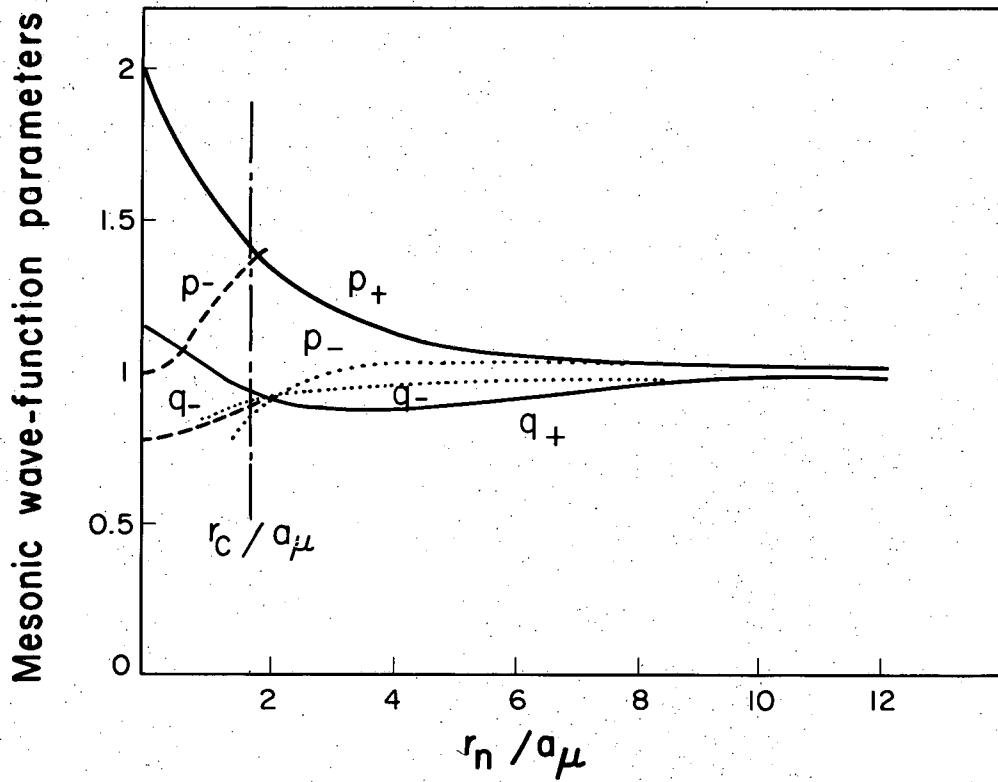
FIGURE LEGENDS

- Fig. 1. Static molecular-ion potentials for the lowest symmetric (W_+) and antisymmetric (W_-) mesonic states. Here \square indicates values obtained by Teller,⁴ and \odot the exact values of Hylleras.⁴
- Fig. 2. Mesonic wave-function parameters, $p_{\pm}(r) = P_{\pm}(r)/r$ and $q_{\pm}(r) = Q_{\pm}(r)/r$, which minimize the static Hamiltonian. For the antisymmetric states, different curves are presented for $r < r_c$, $r > r_c$ (see text).
- Fig. 3. First-order dynamic corrections to the molecular-ion potentials for the equal-mass case.
- Fig. 4. First-order dynamic correction terms to the molecular-ion potentials for the unequal-mass case ($m_1/m_2 = 2$).
- Fig. 5. First-order dynamic coupling terms between the lowest symmetric and antisymmetric molecular-ion states for the unequal-mass case ($m_1/m_2 = 2$).



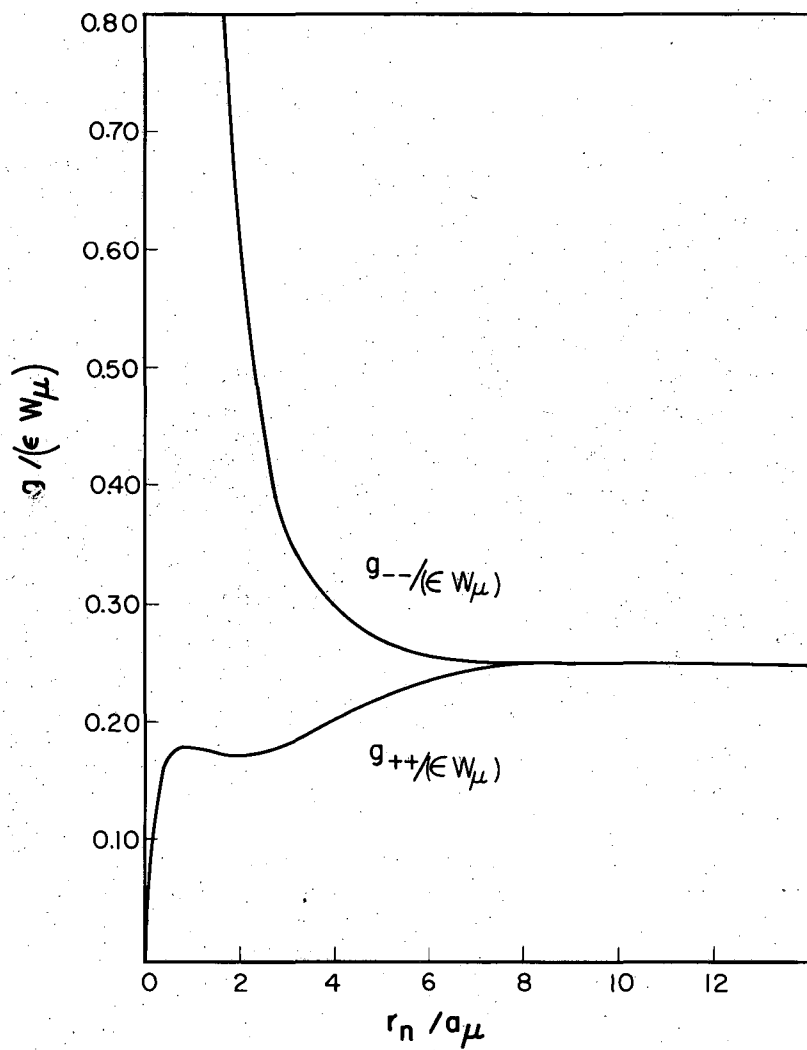
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Fig. 1



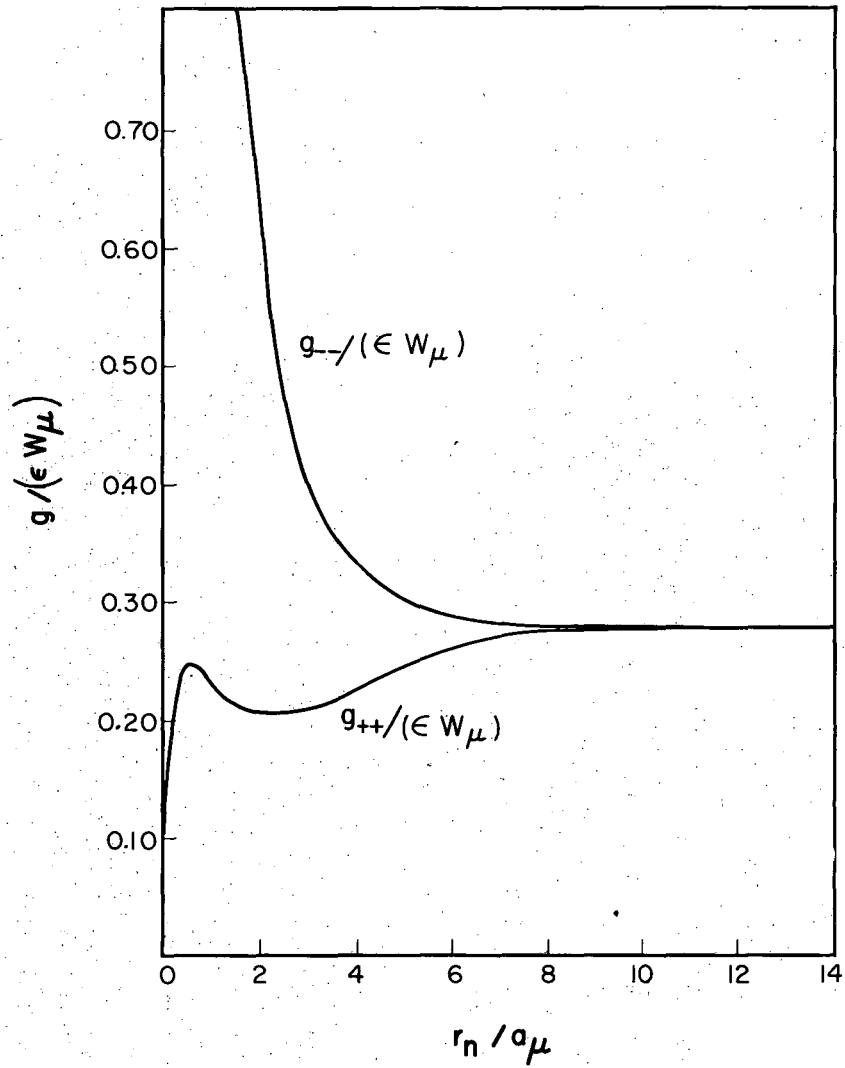
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Fig. 2



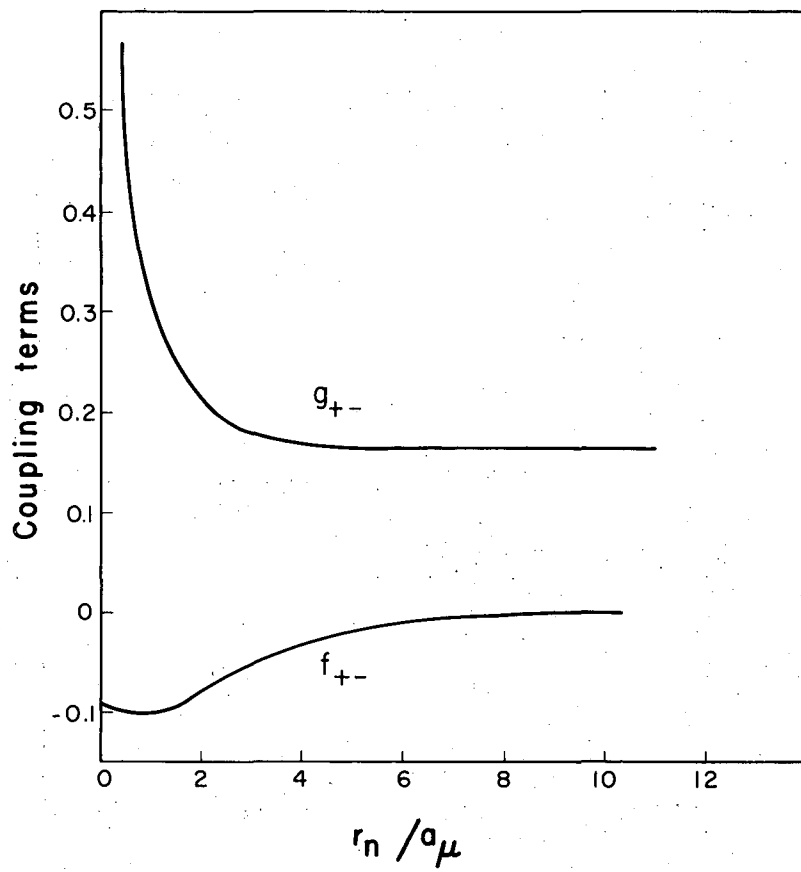
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Fig. 3¹¹



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Fig. 4



MU-17375

Fig. 5

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