

Configuration space Faddeev continuum calculations: p-d *s*-wave scattering length

J. L. Friar and B. F. Gibson

Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545

G. L. Payne

Department of Physics and Astronomy, University of Iowa, Iowa City, Iowa 52242

(Received 31 May 1983)

Formulation of *s*-wave zero-energy Faddeev-type scattering equations including a Coulomb interaction is discussed. Numerical solutions of these equations for the *s*-wave NN potential models of Malfliet and Tjon are obtained using spline techniques. Kohn variational estimates are presented and comparison is made to previously published results. Our quartet pd scattering lengths are larger than others previously obtained, and our pd doublet results are smaller than the corresponding nd results, and thus in contrast to the experimental values. An explication of this feature is presented in terms of a model two-body problem. Perturbation theory for the Coulomb corrections to the scattering length is developed and confirms the Kohn estimates.

[NUCLEAR REACTIONS ${}^2\text{H}(\text{p,p}){}^2\text{H}$, $E=0$ MeV, p-d *s*-wave scattering lengths,
configuration space Faddeev calculations.]

I. INTRODUCTION

Two of the primary reasons for performing calculations with exact few-body equations are to probe for novel features of physical observables and to test our understanding of nuclear forces by direct comparison with data. Trinucleon bound state investigations have yielded important results in each category. For an attractive two-body potential, the interaction becomes more attractive in a two-body system as well as in a three-body system when the scattering length becomes larger; however, as the effective range becomes larger the interaction becomes more attractive in the two-body system but less attractive in the three-body system.¹ This effect was, in fact, the basis of the early argument that nucleon-nucleon forces are not of zero range: Thomas showed that a zero-range attractive force would lead to infinite binding energy for the triton.^{2,3} Total binding energies and binding energy differences are two of the most precisely determined quantities in nuclear physics. The ${}^3\text{H}$ - ${}^3\text{He}$ binding energy difference provides a test of our understanding of Coulomb forces, charge symmetry breaking, neutron-proton mass difference effects, etc.⁴⁻⁸ Nevertheless, it is the scattering problem which offers us the opportunity to explore in depth the accuracy of our knowledge of the nucleon-nucleon force. Neutron-deuteron (nd) elastic scattering at zero incident energy is the simplest three-nucleon scattering problem in physics. In spite of this, it was several years after Faddeev's revolutionary work⁹ on the *t*-matrix approach to the solution of the three-body scattering problem that the correct experimental nd quartet (${}^4a_{\text{nd}}$) and doublet (${}^2a_{\text{nd}}$) *s*-wave scattering lengths were determined from the competing possibilities.¹⁰⁻¹²

Pursuit of a solution to this dilemma concerning the correct choice of nd scattering lengths led to the discovery

of an interesting linear relationship between the nd doublet scattering length and the triton binding energy $B({}^3\text{H})$. First emphasized by Phillips,¹³ this relationship was explicitly noted as being the result of a pole in the scattering amplitude by several authors^{10,14-16}

$$k \cot \delta = \left[-\frac{1}{a} + \frac{1}{2}r_0k^2 + Pk^4 \right] / (1 + k^2/aR)$$

$$= R(-1 + \frac{1}{2}ar_0k^2 + aPk^4)/(aR + k^2). \quad (1)$$

It is clear that $k \cot \delta$ has a pole at $k^2 = -aR$, and that the pole position (corresponding to the bound state of ${}^3\text{H}$) varies linearly with the scattering length a , near that pole. It has since been demonstrated numerically that most nucleon-nucleon potential models produce values of ${}^2a_{\text{nd}}$ and $B({}^3\text{H})$ which fall along the Phillips line whenever the triplet potential reproduces the correct binding energy of the deuteron.¹⁷ It was in part the intuition gained from this simple linear relationship based upon short-range, two-body forces (as the binding energy of the triton is reduced, the magnitude of the doublet scattering length is increased) that led to the general acceptance of the *s*-wave proton-deuteron (pd) quartet and doublet scattering length values determined from phase shift analyses of the available low-energy pd elastic scattering data,^{10,18}

$${}^4a_{\text{pd}} = 11.88_{-0.1}^{+0.4} \text{ fm},$$

$${}^2a_{\text{pd}} = 2.73 \pm 0.10 \text{ fm}. \quad (2)$$

These are to be compared with nd values of ${}^4a_{\text{nd}} = 6.4$ fm and ${}^2a_{\text{nd}} = 0.65$ fm. The sign and approximate magnitude of the quartet difference ${}^4a_{\text{pd}} - {}^4a_{\text{nd}}$ have been reproduced by several theoretical calculations.¹⁹⁻²² The estimate of ${}^4a_{\text{pd}} = 13.3$ fm by Alt²² in a separable potential model

study is the only one of these estimates which is significantly larger than the experimental value. The Jost function approximation procedure of Timm and Stingl,¹⁹ the dispersion relation approach of Eyre, Phillips, and Roig,²⁰ and the approximation procedure of Avishai and Rinat²¹ all estimated values of $^4a_{pd}$ in agreement with the quoted experimental result. The doublet estimates of Refs. 20 and 21 also agree qualitatively with the experimental value of $^2a_{pd}$, implying a large increase in the magnitude of the doublet scattering length when a Coulomb force is present.

Our calculations based upon configuration space Faddeev equations and (partial-wave) local s -wave nucleon-nucleon interactions suggest that the experimental s -wave pd scattering lengths should be reevaluated. In particular, we make the following points:

(1) We find $^4a_{pd}$ to be approximately 14 fm, in reasonable agreement with the Alt-Grassberger-Sandhas (AGS) equation estimate of Alt for a separable model with no short-range repulsion.

(2) We find $^2a_{pd}$ to be approximately zero, in contradiction to intuitive estimates based upon experience with the Phillips line; our value of $^2a_{pd}$ is smaller than $^2a_{nd}$, rather than larger.

This novel feature of the "Coulomb correction" to the doublet scattering length is, in fact, analogous to the Coulomb corrections in a corresponding two-body problem, as we will demonstrate. In addition, our large quartet scattering length is confirmed by perturbation theory estimates. Therefore, our results are readily understandable.

In Sec. II of this paper we review the three-body scattering equations in configuration space. We choose to work in configuration space because we wish to explore the three-body continuum wave functions and because the long-range Coulomb interaction is naturally introduced in that space. In Sec. III we discuss the numerical solution of the partial-wave equations including the important boundary condition question. In Sec. IV we discuss our numerical results and present graphically the differences in the wave functions resulting from the choice of equations to be solved. In Sec. V we discuss the relationship of our predictions to scattering lengths in the two-body potential problem. We summarize our conclusions in Sec. VI.

II. FADDEEV EQUATIONS IN CONFIGURATION SPACE: MODIFIED EQUATIONS

The zero incident energy in a non-Coulomb scattering length calculation dictates that only amplitudes coupling to $\mathcal{L}=0$ open channels are required, where \mathcal{L} is the total orbital angular momentum of the system. The Malfliet-Tjon potential²³ acts only in the s wave; i.e., one has a nonzero force only for $l=0$ interacting pairs. Therefore, in our nd scattering length investigations,²⁴ only the $l=0$, $L=0$, $\mathcal{L}=0$ partial wave of the Faddeev amplitude was nonzero. (The $l=0$ interaction implies that the angular momentum L of the spectator must also be zero.) The size of the numerical calculations is considerably reduced when the Faddeev amplitude is restricted to the $l=0$, $L=0$ partial wave. Nevertheless, the Schrödinger wave function

does include higher partial waves which arise from the permuted terms of the Faddeev amplitude. For a short-range interaction the approximation of limiting the number of partial waves gives reasonably accurate solutions. The Coulomb potential is not a short-range interaction. Thus, one must either explicitly include more partial waves or else modify the Faddeev equations so that the effective interaction has a short range. We choose to follow the latter approach. The possibility of using modified equations has been suggested by Redish.²⁵ Sasakawa and Sawada²⁶ studied the particular case of the Coulomb potential. The techniques described in this paper are similar to those used for our ^3He bound state calculation.⁸ In this section we present a general derivation. We define three different ways in which to modify the Faddeev equations when a Coulomb force is included. In Sec. IV we present numerical results for these three choices of the modified Faddeev equations. We restrict ourselves to the s -wave scattering solutions.

As in our previous studies^{8,24,27} we decompose the Schrödinger equation into the three coupled Faddeev equations

$$[T + V(\vec{x}_i) - E]\psi(\vec{x}_i, \vec{y}_i) = -V(\vec{x}_i)[\psi(\vec{x}_j, \vec{y}_j) + \psi(\vec{x}_k, \vec{y}_k)], \quad (3)$$

where T is the kinetic energy operator and $V(\vec{x}_i)$ is the two-body potential representing the *nuclear-plus-Coulomb* interaction between particles j and k . The Schrödinger wave function is given by

$$\begin{aligned} \Psi &= \psi(\vec{x}_1, \vec{y}_1) + \psi(\vec{x}_2, \vec{y}_2) + \psi(\vec{x}_3, \vec{y}_3) \\ &\equiv \psi_1 + \psi_2 + \psi_3, \end{aligned} \quad (4)$$

where we have used the Jacobi coordinates

$$\vec{x}_i = \vec{r}_j - \vec{r}_k, \quad (5)$$

$$\vec{y}_i = \frac{1}{2}(\vec{r}_j + \vec{r}_k) - \vec{r}_i,$$

for particles with coordinates \vec{r}_i , \vec{r}_j , and \vec{r}_k . The two-body potentials have the form

$$V(\vec{x}_i) = V_N(\vec{x}_i) + \frac{e^2}{x_i} P_C^{j,k}, \quad (6)$$

where V_N is the strong nuclear potential and

$$P_C^{j,k} = \frac{1}{4}(1 + \tau_j^z)(1 + \tau_k^z) \quad (7)$$

is the charge projection operator. Because $V(\vec{x}_i)$ contains the long-range Coulomb potential, the coupling to the higher partial waves in Eq. (3) cannot be neglected. However, Eq. (3) can be modified by adding terms to the three coupled equations, such that the coupling terms on the right-hand side of Eq. (3) fall off faster than $1/y$ and the sum of the three equations is still the Schrödinger equation. That is, we rewrite Eq. (3) in the form

$$\left[T + V_N(\vec{x}_i) + \frac{e^2}{x_i} P_C^{j,k} + W_j(\vec{x}_i, \vec{y}_i) P_C^{k,i} + W_k(\vec{x}_i, \vec{y}_i) P_C^{i,j} - E \right] \psi(\vec{x}_i, \vec{y}_i) \\ = - \left[V_N(\vec{x}_i) + \frac{e^2}{x_i} P_C^{j,k} - W_i(\vec{x}_j, \vec{y}_j) P_C^{i,k} \right] \psi(\vec{x}_j, \vec{y}_j) - \left[V_N(\vec{x}_i) + \frac{e^2}{x_i} P_C^{j,k} - W_i(\vec{x}_k, \vec{y}_k) P_C^{i,k} \right] \psi(\vec{x}_k, \vec{y}_k), \quad (8)$$

where the W_i are arbitrary.

For the choice

$$W_i(\vec{x}_j, \vec{y}_j) = e^2/y_j, \quad (9)$$

the equations reduce to the form used in our ^3He bound state calculations. For this case the coupling terms on the right-hand side of Eq. (8) fall off as $1/y_j^2$ ($1/y_k^2$) for large values of y_j (y_k). Thus, the coupling to higher partial waves is reduced. We emphasize that the left-hand side of Eq. (8) contains the long-range Coulomb distortion effects because of the terms which are proportional to $1/y_i$.

A second choice for the W_i is

$$W_i(\vec{x}_j, \vec{y}_j) = \frac{e^2}{x_i}. \quad (10)$$

For this choice the Coulomb terms on the right-hand side of Eq. (8) cancel completely. On the left-hand side of Eq. (8), one has the Coulomb distortion terms of the form

$$\frac{e^2}{x_j} = \frac{e^2}{|\vec{y}_i - \vec{x}_i/2|} = e^2 \sum_{n=0}^{\infty} \frac{r_{<}^n}{r_{>}^{n+1}} P_n(\mu), \quad (11)$$

where $r_{<}$ ($r_{>}$) is the lesser (greater) of y_i and $x_i/2$, and μ is the cosine of the angle between \vec{x}_i and \vec{y}_i . In this case, restricting the Faddeev amplitude to the $l=0$ partial wave corresponds to replacing a part of the Coulomb interaction by $e^2/r_{>}$; that is, we neglect a small part of the Coulomb potential which has a short range.

From the discussion above one can see that an obvious third choice for W_i is simply

$$W_i = e^2/r_{>} \quad (12)$$

in all partial waves. For this choice, the Coulomb coupling terms on the right-hand side of Eq. (8) are not identically zero but will fall off as $1/y_j^2$ ($1/y_k^2$) for large values of y_j (y_k).

Of these three possible modifications of the Faddeev equations, that defined by Eq. (10) is optimal. The long range Coulomb coupling on the right-hand side of Eq. (8) vanishes, which makes the $l=0$ approximation for the Faddeev amplitude work best. This will be demonstrated numerically in Sec. IV, where scattering lengths from Faddeev solutions and Kohn variational procedures are compared.

III. NUMERICAL METHODS

Because we restrict our consideration to s -wave strong interactions, the quartet ($J = \frac{3}{2}$) system is described by a single Faddeev amplitude and the doublet ($J = \frac{1}{2}$) system is described by a total of two Faddeev amplitudes. (We neglect the small $T = \frac{3}{2}$ admixture to the wave function in this discussion.) We write these amplitudes as

$$\psi_{i=0}^{l=0}(\vec{x}_i, \vec{y}_i) = \frac{\phi(x_i, y_i)}{x_i y_i} \chi_3(i; j, k) \eta_1(i; j, k) \quad (13)$$

for the quartet case and

$$\psi_{i=0}^{l=0}(\vec{x}_i, \vec{y}_i) = \frac{\phi_s(x_i, y_i)}{x_i y_i} \chi_2(i; j, k) \eta_1(i; j, k) \\ + \frac{\phi_t(x_i, y_i)}{x_i y_i} \chi_1(i; j, k) \eta_2(i; j, k) \quad (14)$$

for the doublet case. The ϕ are the reduced Faddeev amplitudes having $l=L=\mathcal{L}=0$. The χ (η) are the spin (isospin) functions defined by Schiff.²⁸ Specifically, the spin functions are

$$\chi_1 = (\frac{1}{2}, 1)_{\frac{1}{2}}, \\ \chi_2 = (\frac{1}{2}, 0)_{\frac{1}{2}}, \\ \chi_3 = (\frac{1}{2}, 1)_{\frac{3}{2}}, \quad (15)$$

and the isospin functions are

$$\eta_1 = (\frac{1}{2}, 1)_{\frac{1}{2}}, \\ \eta_2 = (\frac{1}{2}, 0)_{\frac{1}{2}}. \quad (16)$$

The numerical solution of the Faddeev equations is considerably simplified if one removes the known structures from the ϕ functions.²⁴ For the quartet amplitude we define $F(x_i, y_i)$ according to

$$\phi(x_i, y_i) = [y_i \mathcal{S}(x_i) - F(x_i, y_i) \mathcal{K}(y_i)] u_d(x_i), \quad (17)$$

where u_d is the deuteron bound-state wave function. The \mathcal{S} and \mathcal{K} functions are defined in terms of the modified Bessel function I_1 and K_1 with arguments

$$z_i = 2 \frac{e^2}{\hbar^2} \mu_{jk, i} y_i = \frac{4}{3} \frac{M \alpha c}{\hbar} y_i; \\ \mathcal{S}(y_i) = I_1(2\sqrt{z_i}) / \sqrt{z_i}, \quad (18) \\ \mathcal{K}(y_i) = 2\sqrt{z_i} K_1(2\sqrt{z_i}). \quad (19)$$

The quantity $\mu_{jk, i}$ is the reduced mass of particle i and the bound jk pair. We use $\hbar^2/M = 41.47 \text{ MeV fm}^2$ throughout. Note that both

$$\mathcal{S}(y_i) \xrightarrow{\alpha \rightarrow 0} 1$$

and

$$\mathcal{K}(y_i) \xrightarrow{\alpha \rightarrow 0} 1$$

as the Coulomb interaction ($\alpha = e^2/\hbar c$) is turned off, so that one recovers the amplitude for nd scattering.²⁴

For the doublet case we define $F_s(x_i, y_i)$ and $F_t(x_i, y_i)$ according to

$$\phi_s(x_i, y_i) = F_s(x_i, y_i) \quad (20)$$

and

$$\phi_t(x_i, y_i) = [y_i \mathcal{S}(y_i) - F_t(x_i, y_i) \mathcal{K}(y_i)] u_d(x_i). \quad (21)$$

It is only necessary to remove the deuteron and asymptotic structures from the amplitude in which the interacting pair is in a triplet state. Again these amplitudes reduce to those of Ref. 24 when the Coulomb interaction vanishes.

The integrodifferential equation for the quartet function $F(x_1, y_1)$ is

$$\begin{aligned} u_d(x_1) \mathcal{K}(y_1) \left[\frac{\partial^2}{\partial x_1^2} + \frac{3}{4} \frac{\partial^2}{\partial y_1^2} \right] F(x_1, y_1) + 2 \mathcal{K}(y_1) \frac{du_d}{dx_1} \frac{\partial F}{\partial x_1} + \frac{3}{2} u_d(x_1) \frac{d\mathcal{K}}{dy_1} \frac{\partial F}{\partial y_1} \\ + u_d(x_1) \mathcal{K}(y_1) [U_C(y_1) - U_D(x_1, y_1)] F(x_1, y_1) + \frac{1}{2} U_t(x_1) \int_{-1}^1 d\mu \frac{x_1 y_1}{x_2 y_2} u_d(x_2) \mathcal{K}(y_2) F(x_2, y_2) \\ = [U_C(y_1) - U_D(x_1, y_1)] y_1 \mathcal{S}(y_1) u_d(x_1) + \frac{1}{2} U_t(x_1) \int_{-1}^1 d\mu \frac{x_1 y_1}{x_2 y_2} y_2 u_d(x_2) \mathcal{S}(y_2). \quad (22) \end{aligned}$$

Here μ is the cosine of the angle between \vec{x}_1 and \vec{y}_1 ,

$$U_C(y) = \frac{M \alpha c}{\hbar} \frac{1}{y},$$

$$U_D(x, y) = \frac{M}{\hbar^2} W_{l=0}(\vec{x}, \vec{y}),$$

and

$$U_t(x) = \frac{M}{\hbar^2} V_t(x).$$

Note that if $W(\vec{x}, \vec{y})$ is not explicitly $1/y$, then the scattering length will not vanish identically when one sets $V_t(x) \equiv 0$. We shall return to the point in Sec. IV.

The coupled equations to be solved for $F_s(x_i, y_i)$ and $F_t(x_i, y_i)$ are the following ($\kappa^2 = -ME_d/\hbar^2$, where E_d is the deuteron binding energy):

$$\begin{aligned} \left[\frac{\partial^2}{\partial x_1^2} + \frac{3}{4} \frac{\partial^2}{\partial y_1^2} - \kappa^2 \right] F_s(x_1, y_1) - U_s(x_1) \left\{ F_s(x_1, y_1) + \int_{-1}^1 d\mu \frac{x_1 y_1}{x_2 y_2} \left[\frac{1}{4} F_s(x_2, y_2) + \frac{3}{4} u_d(x_2) \mathcal{K}(y_2) F_t(x_2, y_2) \right] \right\} \\ - \left[\frac{2}{3} U_C(x_1) + \frac{1}{3} U_D(x_1, y_1) \right] F_s(x_1, y_1) - \frac{2}{3} \int_{-1}^1 d\mu \frac{x_1 y_1}{x_2 y_2} [U_C(x_1) - U_D(x_2, y_2)] \left[\frac{1}{4} F_s(x_2, y_2) + \frac{3}{4} u_d(x_2) \mathcal{K}(y_2) F_t(x_2, y_2) \right] \\ = -\frac{3}{4} U_s(x_1) \int_{-1}^1 d\mu \frac{x_1 y_1}{y_2 y_2} y_2 u_d(x_2) \mathcal{S}(y_2) - \frac{1}{2} \int_{-1}^1 d\mu \frac{x_1 y_1}{x_2 y_2} [U_C(x_1) - U_D(x_2, y_2)] y_2 u_d(x_2) \mathcal{S}(y_2) \quad (23) \end{aligned}$$

and

$$\begin{aligned} u_d(x_1) \mathcal{K}(y_1) \left[\frac{\partial^2}{\partial x_1^2} + \frac{3}{4} \frac{\partial^2}{\partial y_1^2} \right] F_t(x_1, y_1) + 2 \mathcal{K}(y_1) \frac{du_d}{dx_1} \frac{\partial F_t}{\partial x_1} + \frac{3}{2} u_d(x_1) \frac{d\mathcal{K}}{dy_1} \frac{\partial F_t}{\partial y_1} + [U_C(y_1) - U_D(x_1, y_1)] \\ \times u_d(x_1) \mathcal{K}(y_1) F_t(x_1, y_1) - U_t(x_1) \int_{-1}^1 d\mu \frac{x_1 y_1}{x_2 y_2} \left[\frac{3}{4} F_s(x_2, y_2) + \frac{1}{4} u_d(x_2) \mathcal{K}(y_2) F_t(x_2, y_2) \right] \\ = [U_C(y_1) - U_D(x_1, y_1)] y_1 u_d(x_1) \mathcal{S}(y_1) - \frac{1}{4} U_t(x_1) \int_{-1}^1 d\mu \frac{x_1 y_1}{x_2 y_2} y_2 u_d(x_2) \mathcal{S}(x_2). \quad (24) \end{aligned}$$

Actual numerical calculations were performed by making the standard change of variables to the ρ - θ coordinates,^{24,27} which are defined by

$$x_1 = \rho \cos \theta, \quad (25a)$$

$$y_1 = \frac{\sqrt{3}}{2} \rho \sin \theta. \quad (25b)$$

The $F(\rho, \theta)$ functions are expressed in terms of bicubic splines on a rectangular grid of these ρ - θ coordinates. The coefficients of the splines are obtained using the method of orthogonal collocation.²⁷ We take advantage of the fact that the knots of the splines do not have to be equally spaced. The function $F(\rho, \theta)$ varies slowly for larger values of ρ . We break ρ into two regions, $(0, \rho_{br})$ and (ρ_{br}, ρ_{max}) . We use a uniform distribution of splines between ρ_{br} and ρ_{max} but scale by the factor S_ρ inside ρ_{br}

such that

$$(\rho_{n+1} - \rho_n) = (\rho_n - \rho_{n-1}) S_\rho .$$

In the θ variable we use a uniform distribution between 0 and $\pi/6$ but scale as for ρ between $\pi/6$ and $\pi/2$.

Using standard Green's function techniques, it can be shown that the reduced quartet amplitude has the asymptotic form

$$\phi(x_i, y_i) \xrightarrow{y_i \rightarrow \infty} [y_i \mathcal{S}(y_i) - {}^4 a \mathcal{K}(y_i)] u_d(x_i) . \quad (26)$$

That is, the scattering length is the asymptote of the function $F(x_i, y_i)$. Similarly, for the doublet case, the asymptotic forms of the reduced amplitudes for large values of y_i are

$$\phi_s(x_i, y_i) \xrightarrow{y_i \rightarrow \infty} 0 , \quad (27a)$$

$$\phi_t(x_i, y_i) \xrightarrow{y_i \rightarrow \infty} [y_i \mathcal{S}(y_i) - {}^2 a \mathcal{K}(y_i)] u_d(x_i) . \quad (27b)$$

For all of the reduced amplitudes, the boundary condition for large values of x_i is

$$\phi(x_i, y_i) \xrightarrow{x_i \rightarrow \infty} 0 . \quad (28)$$

These boundary conditions along with

$$\phi(0, y_i) = \phi(x_i, 0) = 0 \quad (29)$$

for all reduced amplitudes provide a unique solution for both the quartet and doublet Faddeev equations.

As a further check on the accuracy of our solution, we make Kohn variational estimates of the scattering lengths utilizing the wave functions obtained as solutions to the Faddeev equations. A complete discussion of the derivation of the Kohn estimates can be found in Ref. 24. The

TABLE I. Potential parameters for the Malfliet-Tjon, Yukawa, and exponential models studied.

Model	V_A (MeV fm)	μ_A (fm ⁻¹)	V_R (MeV fm)	μ_R (fm ⁻¹)
MT I	513.968	1.550	1438.720	3.110
MT III	626.885	1.550	1438.720	3.110
MT IV	65.120	0.633	0	
Yuk _s (AAV)	56.3653	0.863	0	
Yuk _t (AAV)	70.7476	0.712	0	
	(MeV)		(MeV)	
Exp _s (AAV)	111.4584	1.415	0	
Exp _t (AAV)	181.7537	1.453	0	

addition of a Coulomb force does not alter the procedure except in that we calculate two different scattering length estimates, one with an s -wave projected Coulomb potential and one with the full Coulomb interaction.

IV. NUMERICAL RESULTS

We study in detail the stability, convergence, and accuracy of our configuration space solution to the zero-energy scattering length problem utilizing the Malfliet-Tjon²³ singlet and triplet s -wave potentials I and III (the MT I-III model). These partial-wave local two-body potentials are sums of Yukawa forms exhibiting a long-range attraction and a short-range repulsion,

$$V(r) = (V_R e^{-\mu_R r} - V_A e^{-\mu_A r}) / r . \quad (30)$$

The parameters of the MT I-III model are listed in Table I along with those of the MT IV (purely attractive potential) model. Parameters for Yukawa and exponential

TABLE II. Mesh parameters used in the accuracy and convergence study of the pd scattering length calculations using the MT I-III potential model.

Case	N_I^p	N_E^p	ρ_{br}	S_ρ	ρ_{max}	N_I^g	N_E^g	S_θ
1	18	12	15.	1.3	80.	20	6	1.3
2	15	12	12.	1.3	80.	20	6	1.3
3	15	12	10.	1.3	70.	20	6	1.3
4	15	12	10.	1.3	80.	14	6	1.3
5	15	12	10.	1.3	80.	20	6	1.2
6	15	12	10.	1.3	80.	20	6	1.4
7	15	12	10.	1.2	80.	20	6	1.3
8	12	8	10.	1.3	70.	16	4	1.3
9	12	8	10.	1.3	70.	18	2	1.3
10	10	10	10.	1.3	58.	18	2	1.3
11	14	12	12.	1.3	82.	18	6	1.3
12	14	12	12.	1.3	82.	16	4	1.3
13	14	8	12.	1.3	82.	16	4	1.3
14	10	10	12.	1.3	82.	16	4	1.3
15	10	8	12.	1.3	68.	16	4	1.3
16	10	10	12.	1.4	82.	16	4	1.3
17	10	10	12.	1.3	82.	16	4	1.4
18	10	10	10.	1.3	82.	16	4	1.3
19	10	10	15.	1.3	82.	16	4	1.3
20	14	12	15.	1.3	82.	17	3	1.3

$(-V_A e^{-\mu_A r})$ potentials fitted to the separable potential scattering lengths and effective ranges of Aaron, Amado, and Yam²⁹ (AAY) are also listed for our comparison with the quartet scattering length result of Alt.²²

As was the case in our study²⁴ of the nd scattering lengths we consider the MT I-III model in greatest detail. We list in Table II the mesh parameter values for a selection of the test cases run for the quartet and doublet pd scattering lengths. In Table III we provide the value extracted from the asymptotic wave function and the corresponding Kohn variational estimate (a^K) based upon that wave function and an s -wave projected Coulomb potential. In all cases we have used the modified Faddeev equation corresponding to the choice of Eq. (10) in Sec. II. That is, we have selected the case in which there is no Coulomb coupling on the right-hand side of Eq. (8), the choice in which

$$U_D(x_i, y_i) = \frac{M\alpha c}{\hbar} \frac{1}{|\vec{y}_i \mp \vec{x}_i/2|} \Big|_{l=0}$$

in Eqs. (22)–(24). Note that, as remarked above, 4a and 2a do not vanish for this choice of W_i when the strong potential vanishes. However, ${}^4a(V_i \equiv 0) \leq 0.005$ fm, so that a correction for this effect is smaller than the numerical uncertainty of our solution.

As was true in our study of the bound state, the sensitivity of the solution to the ρ -grid parameters proved to be the more complex. Convergence with respect to the cutoff radius ρ_{\max} was obtained by about 80 fm, somewhat larger than in the case of nd scattering, as one would expect. A ρ_{br} value of between 10 and 12 fm was again optimal. As

TABLE III. MT I-III model quartet and doublet scattering lengths along with the s -wave projected and full Kohn estimates for the mesh parameters listed in Table I. Units are fm.

Case	4a	${}^4a^K$	${}^4a^{K,F}$
1	13.765	13.766	13.962
2	13.766	13.766	13.962
3	13.765	13.766	13.962
4	13.627	13.766	13.962
5	13.735	13.766	13.962
6	13.767	13.766	13.962
7	13.764	13.766	13.962
8	13.749	13.765	13.960
9	13.762	13.765	13.960
10	13.753	13.754	13.950
	2a	${}^2a^K$	${}^2a^{K,F}$
11	0.1543	0.1555	0.0031
12	0.1648	0.1555	0.0031
13	0.1638	0.1557	0.0033
14	0.1639	0.1566	0.0043
15	0.1648	0.1569	0.0045
16	0.1629	0.1569	0.0046
17	0.1492	0.1566	0.0043
18	0.1588	0.1565	0.0041
19	0.1629	0.1579	0.0055
20	0.1539	0.1555	0.0031

for the nd problem, the number of splines (N_I) in the interior region must be 10–12 to provide a reasonable solution, and the scale factor S_ρ should lie between 1.2 and 1.4. In the exterior region, where the wave function is relatively smooth, a uniform spacing of as large as 6–7 fm is feasible. At least three θ points uniformly distributed between 0 and $\pi/6$ were needed for a reasonable solution. Scaling the θ distribution between $\pi/6$ and $\pi/2$ such that more points (N_I) lie in the region of the deuteron bound state was important. At least 16 points were needed in that region with a scale factor S_θ of between 1.2 and 1.4.

The difference between the result derived from the asymptotic form of the wave function and the Kohn variational results ($a^{K,F}$) is due primarily to the inclusion of higher partial waves of the Coulomb interaction in the Kohn calculation. That is, there is no s -wave projection in the $a^{K,F}$ results. In contrast, when one uses an s -wave projected Coulomb interaction in the Kohn variational equation, the Kohn results a^K agree well with the values extracted from the asymptotic part of the wave function. Thus, our best estimates of the quartet and doublet s -wave projected scattering length values are 13.76 ± 0.01 fm and 0.15 ± 0.01 fm. Our best estimate of the physical scattering lengths, including all partial waves by means of the Kohn variational procedure, are 13.96 ± 0.01 fm and 0.003 ± 0.002 fm.

Let us turn our attention to the question of comparing results from the three different Coulomb modification procedures defined in Sec. II. In Table IV we list 2a results extracted from the wave function and results estimated via the Kohn procedure. It is clear that failure to remove the higher partial-wave Coulomb coupling from the right-hand side of Eq. (8) has a non-negligible effect when one then imposes an s -wave projection on the solution. However, it is also clear from the ${}^2a^{K,F}$ results that the complete Schrödinger wave function comes very close to producing the right estimate of 2a for all three procedures. The effect on the wave function of having a long range coupling on the right-hand side of Eq. (8) can be seen by comparing F_s amplitudes in Figs. 1 and 2. In Fig. 1, F_s obtained using the e^2/x_i choice for W_i vanishes smoothly at large distances. In Fig. 2, F_s obtained with the e^2/r choice for W_i still shows significant structure out to ρ_{\max} . (F_x from e^2/y_j shows the same structure in the asymptotic region.) Thus, removal of long-range coupling to the higher partial waves is important in generating an accurate solution of the pd scattering problem.

Although we have not discussed its effect, the amplitude for doublet pd scattering contains a (closed) $T = \frac{3}{2}$ isospin channel. This channel has but a small effect be-

TABLE IV. Comparison of pd doublet scattering lengths using modifications of the Faddeev equations specified by Eqs. (9), (10), and (12). Units are fm.

W_i	2a	${}^2a^K$	${}^2a^{K,F}$
Eq. (9)	-0.4967	-0.5179	0.0366
Eq. (10)	0.1543	0.1555	0.0031
Eq. (12)	-0.5065	-0.5273	0.0151

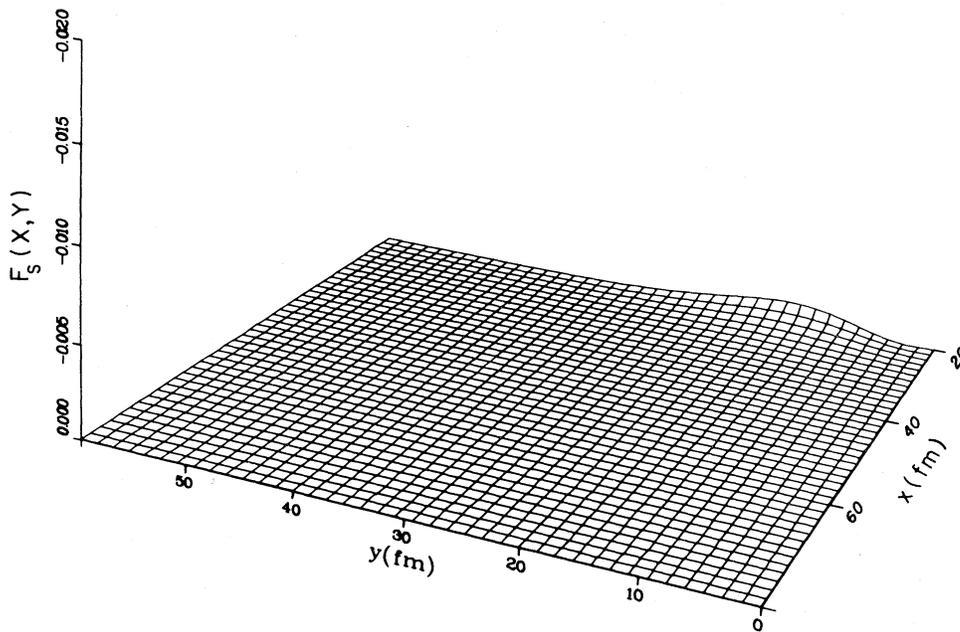


FIG. 1. The function $F_s(x, y)$ using the Coulomb modification corresponding to W_i in Eq. (10); the x coordinate has a suppressed zero.

cause it cannot influence the asymptotic channel in order α . Indeed, it couples only to the closed singlet channel, which produces an α^2 effect in the triplet channel. The smoothness of the Coulomb interaction and the mixed symmetry nature of the isospin impurity are also indicative of a weakly coupled amplitude. Numerically, including the $T = \frac{3}{2}$ channel in the calculation changes ${}^2a_{pd}$ by

approximately 0.008 fm. Neglecting this channel appears to be an excellent approximation.

The only published Faddeev Coulomb calculation for 4a is that of Alt²² using the separable-potential-based AGS formalism.³⁰ He obtained 13.3 fm using the separable potential parameters quoted in Ref. 29. We have generated simple Yukawa and exponential potentials which repro-

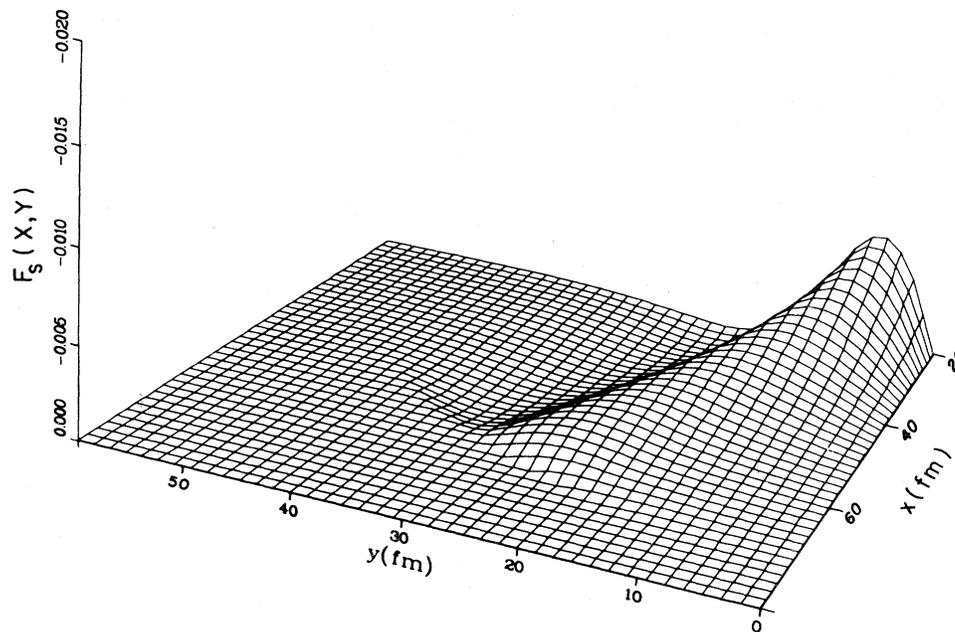


FIG. 2. The function $F_s(x, y)$ using the Coulomb modification corresponding to W_i in Eq. (12); the x coordinate has a suppressed zero.

TABLE V. Comparison of model nd and pd scattering lengths for Yukawa, exponential, and MT potentials with results of Alt. Units are fm.

Model	Alt	Exponential	Yukawa	MT I-III	MT IV
${}^4a_{\text{nd}}$	6.32	6.33	6.39	6.44	6.54
${}^4a_{\text{pd}}$	13.3	13.4	13.6	13.8	14.0
${}^4a_{\text{pd}}^{K,F}$		13.6	13.8	14.0	14.3
${}^2a_{\text{nd}}$		-6.4	-2.1	0.70	
${}^2a_{\text{pd}}$		-7.6	-3.6	0.15	
${}^2a_{\text{pd}}^{K,F}$		-7.8	-3.8	0.003	

duce the two-body scattering lengths and effective ranges of Ref. 29. We compare nd and pd results for 4a and 2a in Table V. Our exponential potential model, which has no $1/r$ singularity, yields a value for 4a in very good agreement with that of Alt. The Yukawa potential 4a result lies half-way between the exponential potential result and that from our MT I-III model calculation. Clearly, the pd quartet scattering length shows minimal sensitivity to the off-shell differences of the purely attractive potentials, although the differences are larger than one sees for the corresponding nd quartet scattering lengths. The inclusion of short-range repulsion leads to a larger Coulomb correction. For completeness, we also provide quartet results for the purely attractive MT IV model. We list the 2a results for the Yukawa and exponential models. We note that in each case 2a becomes more negative when the Coulomb interaction is included. (It is well known that simple potential models overbind the triton and lead to negative values of the nd doublet scattering length.) We return to this in Sec. V. More importantly, we see for the MT I-III model that ${}^2a_{\text{pd}}$ is smaller than ${}^2a_{\text{nd}}$, not larger. This is in disagreement with the observed relationship between the triton binding energy and the nd doublet scattering length, where one sees ${}^2a_{\text{nd}}$ increase as $B({}^3\text{H})$ decreases. The Coulomb force reduces the binding energy of ${}^3\text{He}$ compared to ${}^3\text{H}$, but we also find ${}^2a_{\text{pd}}$ to be less than ${}^2a_{\text{nd}}$.

V. ANALYSIS OF RESULTS

Clearly our pd doublet scattering length result disagrees with both the published experimental values and previous theoretical estimates based upon approximate methods of including Coulomb effects. Also, our pd quartet scattering length result is significantly larger than the experimental value, although it is in reasonable agreement with Alt's.

In order to explicate the results of our calculations, we consider first the zero-energy, two-body problem in which the interaction is the sum of a strong, short-range potential and a Coulomb potential. Asymptotically the wave function has the form

$$\phi(r) \rightarrow r\mathcal{F}(x) - a_C\mathcal{K}(x), \quad (31)$$

$$r \rightarrow \infty$$

where the arguments are related by $x = 2ZZ'\alpha\mu r$. Recall that without a Coulomb force, one has

$$\phi(r) \rightarrow (r - a).$$

$$r \rightarrow \infty$$

Our a_C is the Coulomb modified strong-interaction scattering length; the value would be -7.8 fm for the pp system. By definition, $a_C = 0$ when the strong interaction vanishes and we have only the usual Rutherford scattering. As a concrete example, we choose to work with the MT IV potential. In Fig. 3, we plot the non-Coulomb and Coulomb scattering lengths (a and a_C) as a function of X , an arbitrary strength parameter by which we multiply the potential. [A similar set of curves is obtained when the Reid soft core (RSC) two-body interaction³¹ is utilized.] For negative values of the strength parameter X the two-body interaction is repulsive, whereas for positive values of X the potential is attractive. Both a and a_C vanish at $X = 0$, as they must. Near $X \cong 1.2$ the first bound state appears and the scattering lengths become infinite; the same condition holds at the appearance of the second bound state near $X \cong 5$. For $X < 0$, one finds that $a_C > a$; that is, the Coulomb interaction makes the repulsive strong interaction more repulsive, as anticipated. For $X > 0$ the situation is not quite so simple. Except near $a = 0$, one finds that the curve for a_C is shifted with respect to that for a in such a manner that $a_C > a$. That is, the repulsive Coulomb interaction reduces the attraction of the strong interaction. For example, at $X = 1$ the purely strong interaction result of $a = -17$ fm is modified to a value of

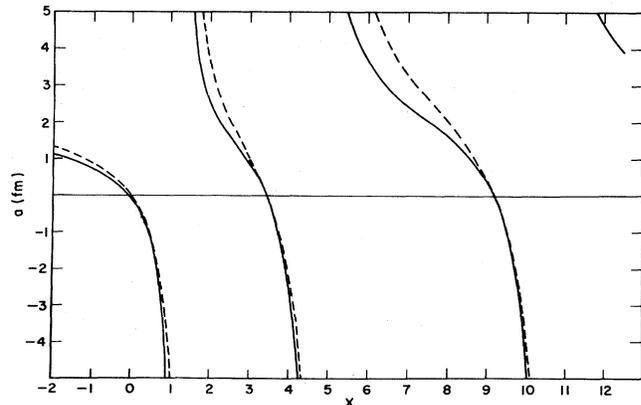


FIG. 3. Two-body scattering lengths a (solid curve) and a_C (dashed curve) as functions of X times the strength of the potential for the MT IV model.

$a_C = -8$ fm. Except for small values of the scattering lengths, the shift in the curve corresponds to the reduction in binding energy due to Coulomb repulsion that one sees, for example, in the binding of ${}^3\text{He}$ compared to the binding of ${}^3\text{H}$.

In Fig. 4 we plot the small region near $a=0$ in order to study the inverted relationship between a and a_C . We display results for both the MT IV and RSC potentials to illustrate the effects of introducing short-range repulsion into the problem. In both cases, we find $a_C < a$ between the crossing points defined by $a = a_C$. This is the reverse of the situation found for most values of X including the familiar case of pp and nn scattering. It lies outside the region of most physical scattering problems, which can be understood in terms of the simple shift in bound state energies due to Coulomb repulsion mentioned above. However, there are physical situations in which experimental scattering lengths are small; a prime example is πN scattering where the scattering lengths are of the order of 0.1 fm.³²

To aid the reader in understanding this property of Coulomb modified strong interactions, we consider the simple rank-one separable potential of the form

$$V(r, r') = \frac{-\Lambda \hbar^2}{2\mu} \frac{1}{4\pi} \frac{e^{-\beta r}}{r} \frac{e^{-\beta r'}}{r'}, \quad (32)$$

where Λ and β are the strength and range of the potential and μ is the two-body reduced mass. The resulting reduced wave function with no Coulomb force is

$$u(r) = f(r) - ag(r), \quad (33)$$

where the two-body Green's function is given by

$$G(r_<, r_>) = -f(r_<)g(r_>).$$

For zero-energy scattering, one has $f(r) = r$ and $g(r) = 1$. The scattering length is given by the well known relationship

$$\begin{aligned} \frac{1}{a} &= - \left[\frac{1}{\Lambda} + \mathcal{F} \right] / \mathcal{L}^2 \\ &= \frac{-\beta^4}{\Lambda} + \frac{\beta}{2}, \end{aligned} \quad (34)$$

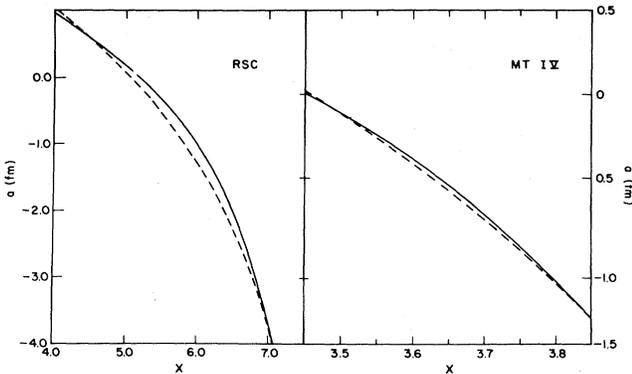


FIG. 4. Two-body scattering lengths a (solid curve) and a_C (dashed curve) as functions of X times the strength of the potential for the RSC and MT IV models.

where the \mathcal{F} and \mathcal{L} integrals are

$$\begin{aligned} \mathcal{F} &= - \int_0^\infty e^{-\beta r} \left[g(r) \int_0^r e^{-\beta r'} f(r') dr' \right. \\ &\quad \left. + f(r) \int_r^\infty e^{-\beta r'} g(r') dr' \right] dr \\ &= \frac{-1}{2} \beta^{-3} \end{aligned} \quad (35)$$

and

$$\begin{aligned} \mathcal{L} &= \int_0^\infty e^{-\beta r} r dr \\ &= \beta^{-2}, \end{aligned} \quad (36)$$

respectively. In the presence of a Coulomb force, the functions become $f(r) = r\mathcal{F}(x)$ and $g(r) = \mathcal{K}(x)$, such that the \mathcal{F} and \mathcal{L} integrals are given by

$$\mathcal{F} = -\beta^{-3} \left[\frac{1}{2} - \frac{\xi}{\beta} e^{2\xi/\beta} E_1(2\xi/\beta) \right] \quad (37)$$

and

$$\mathcal{L} = \beta^{-2} e^{\xi/\beta}, \quad (38)$$

where the exponential integral is

$$E_1(x) = -[\ln(x) + 0.5772 \dots] - \sum_{n=1}^{\infty} \frac{(-)^n x^n}{nn!} \quad (39)$$

and

$$\xi = 2ZZ'\mu\alpha c / \hbar. \quad (40)$$

Thus, the Coulomb modified scattering length³³ is

$$\begin{aligned} \frac{1}{a_C} &= e^{-2\xi/\beta} \left\{ -\beta^4/\Lambda + \beta \left[\frac{1}{2} - \frac{\xi}{\beta} e^{2\xi/\beta} E_1(2\xi/\beta) \right] \right\} \\ &= \frac{1}{a} e^{-2\xi/\beta} - \xi E_1(2\xi/\beta). \end{aligned} \quad (41)$$

To first order in the fine structure constant, the Coulomb modified scattering length a_C and the purely strong interaction scattering length a are simply related by

$$\begin{aligned} \frac{1}{a_C} &\cong \frac{1}{a} (1 - 2\xi/\beta) + \xi [\ln(2\xi/\beta) + 0.5772 \dots] \\ &= \frac{\lambda}{a} + \delta. \end{aligned} \quad (42)$$

Here, λ determines the slope of the curve near $a=0$ and δ represents the shift in the curve discussed above. The fact that $\mathcal{F}(x) > 1$ for all values of r is the reason that we find $\lambda < 1$ for this model; hence, $a_C < a$ in the region near $a \leq 0$. (For a more general discussion see the Appendix.) Therefore, even in this simple separable potential model, we find an illustration of the fact that $a_C > a$ for all situations in which the scattering length a is large enough that the shift δ due to the Coulomb repulsion dominates, whereas for a small region near $a=0$ we have $a_C < a$ due to the properties of the Coulomb function $\mathcal{F}(x)$.

Based upon this brief discussion of the two-body scattering problem involving strong-plus-Coulomb forces, it should be clear that ${}^4a_{pd} > {}^4a_{nd}$, because ${}^4a_{nd} (\cong 6.4 \text{ fm})$

is large. Likewise, one can understand that ${}^2a_{pd} - {}^2a_{nd} \cong 0$, because ${}^2a_{nd} (\cong 0.7 \text{ fm})$ is small. When ${}^2a_{nd}$ is sufficiently small, the actual situation can be ${}^2a_{pd} < {}^2a_{nd}$.

To ensure that these same effects hold for the three-body problem, we have also studied Eq. (22) as a function of X , where X is an arbitrary strength multiplying the strong interaction coupling terms on the right-hand side of the equation. A value of $X=1$ corresponds to the physical quartet problem; a value of $X=-2$ corresponds to a three-boson problem in which two of the particles are charged. Similar behavior was found.

In order to further check our results, we have calculated the change in a_{pd} resulting from the Coulomb interaction in first-order perturbation theory. The details of how this was implemented are discussed in the Appendix. Two sets of calculations were performed for both the quartet and doublet cases. The Coulomb potential was scaled by a dimensionless parameter η , which varied from 0 to 1.2 in steps of 0.1, and the scattering length was calculated for each η using the Faddeev method and the Kohn variational procedure. The Kohn values of a_C/a were fit to various polynomials in η and $\eta \ln \eta$ using the linear least squares approach. Simple low order polynomials were adequate for excellent fits. The linear (in η and $\eta \log \eta$) approximation to these fits was in virtually perfect agreement with the perturbation theory estimate.

An example of this is shown in Fig. 5, where the ratio a_C/a is plotted versus η . For comparison, the linear fits to a_C and $1/a_C$ are shown also. Clearly in this case the latter is the preferable approximation. On this scale there

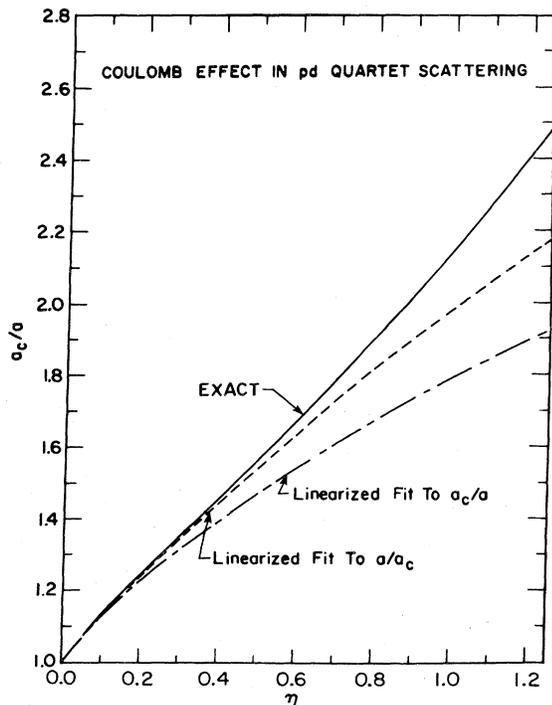


FIG. 5. Comparison for pd quartet scattering of the ratio a_C/a from the exact calculation with perturbation theory expansions for $1/a_C$ and a_C .

is a negligible difference between the linearized fit and perturbation theory. It is rather surprising in view of the large Coulomb shift that first-order perturbation theory works so well and accounts for most of the Coulomb shift.

The doublet scattering length nearly vanishes for $\eta=1$, and this behavior cannot be reproduced using a linear expansion in η for $1/a_C$. Consequently, a linear expansion for a_C works best. These calculations confirm both our Kohn estimates and the essential correctness of our procedure.

VI. CONCLUSIONS

We have calculated the Coulomb modified strong interaction pd scattering lengths using our configuration space formulation of the Faddeev equations. For the s -wave nucleon-nucleon interactions of Malfliet and Tjon (MT I-III), we find ${}^4a_{pd} \cong 14 \text{ fm}$, in reasonable agreement with the AGS equation estimate of Alt using rank-one separable potentials. This is some 2 fm larger than the accepted experimental value. We find ${}^2a_{pd} \cong 0 \text{ fm}$, in disagreement with the accepted experimental value and with intuitive ideas based upon the established linear relation between the triton binding energy and the doublet nd scattering length. Furthermore, we find ${}^4a_{pd}$ and ${}^2a_{pd}$ to be more sensitive to properties of the potential model (off-shell effects) than either ${}^4a_{nd}$, which depends essentially upon only the deuteron binding energy, or ${}^2a_{nd}$, which is determined by the same properties that determine the triton binding energy.

Low-energy pd cross sections are suppressed by the Gamow factor and are therefore difficult to measure accurately. Clearly, further theoretical investigations are in order concerning the correct procedure for extrapolating to zero energy, since this was the source of difficulty in determining the nd scattering lengths. However, the low-energy pd elastic data are not numerous. We hope that these calculations will call to attention the fact that the pd quartet and doublet scattering lengths are just as fundamental as the triton binding energy, the ${}^3\text{H}-{}^3\text{He}$ energy difference, and the nd scattering lengths. As such, they deserve more than the benign neglect which they have recently received.

Note added in proof. Since the completion of this work, a calculation by Kvitsinski [Pis'ma Zh. Eksp. Teor. Fiz. **36**, 375 (1982)] has appeared. Based upon the formalism of Merkuriev [Yad. Fiz. **23**, 6 (1976)], these results are at variance with ours. A recent report by Zankel and Mathelitsch (Nucleon-deuteron low energy parameters, UNIGRAZ-UTP 7/83) confirms our results. For an extensive discussion of the alternative formalisms, the reader should consult Chandler [Nucl. Phys. **A353**, 129c (1981)].

APPENDIX: PERTURBATION THEORY

One of the august techniques used to estimate the size of various physical effects and to check the validity of difficult calculations is perturbation theory, usually limited to first order. To confirm our anomalous results for the shift in the p-d scattering length in the presence of the

Coulomb potential, we have estimated this shift using first-order perturbation theory in the Coulomb interaction. As we will see explicitly below, this perturbation expansion is infinite in each order if performed literally, because the infinite range of the Coulomb force does not produce a sufficient rate of convergence in the necessary integrals. Nevertheless, it is possible to isolate the finite, correct parts of these divergent integrals in a unique way for the following reasons: (1) The integrals over the near-zone part of the scattering wave function are finite; (2) the infinities arise from the asymptotic region of the wave function, whose form is known; (3) consequently, the infinities can be extracted, and the correct finite residue uniquely identified; (4) the analytic results for the separable Yamaguchi model provide an unambiguous check on our procedure. We perform this analysis below for the two body problem; the extension to the three-body (or N -body) problem is trivial.

Motivated by the separable potential result for the Coulomb corrected scattering length a_C , we write our perturbation expansion in the form

$$\frac{1}{a_C} = \frac{\lambda}{a} + \delta \cong \frac{1}{a} + \xi\epsilon + \xi(\ln\xi + 2\gamma), \quad (\text{A1})$$

where γ is Euler's constant and

$$\xi = 2ZZ'\mu\alpha c/\hbar \quad (\text{A2})$$

depends on the proton numbers, Z and Z' , the reduced mass, μ , and the fine structure constant, α . The unknown parameter ϵ can depend on the unperturbed (non-Coulomb) scattering length, a . The dependence of the result on $\ln\xi$ has been assumed, and will be demonstrated below.

The s -wave scattering length wave function has the form

$$\phi(r) = r - ag(r), \quad (\text{A3})$$

where $g(r) \rightarrow [0, 1]$ as $r \rightarrow [0, \infty]$. Perturbation theory yields

$$\begin{aligned} a_C &= 2ZZ' \frac{\mu\alpha c}{\hbar} \int_0^\infty \phi^2(r) \frac{dr}{r} \\ &= \xi \int_0^\infty \left[r - 2ag + a^2 \frac{g^2}{r} \right] dr. \end{aligned} \quad (\text{A4})$$

Every term is divergent, including quadratic, linear, and logarithmic divergences. The quadratic one is simply the "pure Coulomb" scattering length and should be dropped; our result must vanish when a vanishes. The remaining divergences presumably arise because of the peculiarities of the Coulomb corrected s -wave scattering length as defined by³³

$$-\frac{1}{a_C} = \lim_{k \rightarrow 0} [k \cot(\delta_0^c) C_0^2(\xi) + 2\xi kh(\xi)], \quad (\text{A5})$$

where

$$\xi = ZZ'\mu\alpha c/\hbar k = \xi/2k \quad (\text{A6})$$

diverges as the relative momentum k vanishes. The standard auxiliary functions are given by

$$C_0^2(\xi) = 2\pi\xi / (e^{2\pi\xi} - 1) \xrightarrow{\xi \rightarrow 0} 1 - \pi\xi \quad (\text{A7})$$

and

$$\begin{aligned} h(\xi) &= \xi^2 \sum_{m=1}^{\infty} \frac{1}{m(m^2 + \xi^2)} - \ln(\xi) - \gamma \\ &\xrightarrow{\xi \rightarrow 0} -[\ln(\xi) + \gamma], \end{aligned} \quad (\text{A8})$$

where we have approximated each form by its perturbation expansion in $(ZZ'\alpha)$, in spite of the $1/k$ factor. The additional factors in Eq. (A5) are required because δ_0^c is not well behaved; it has linear and logarithmic divergences in $1/k$. Thus, we can presume that the divergences in Eq. (A4) are isomorphs of the one in Eqs. (A7) and (A8).

We therefore calculate at very tiny k , and develop our perturbation expansion. To the order we work it suffices to expand all expressions involving phase shifts to first order. We write $\delta_0^c/k \equiv -\tilde{a}_C(k)$, $\delta_0/k = -a$, and use the standard DWBA expression

$$\tilde{a}_C \cong a + \xi \int_R^\infty \phi^2(r) \frac{dr}{r} + \xi \int_0^R \phi^2(r) \frac{dr}{r}, \quad (\text{A9})$$

where

$$\phi(r) = \frac{\sin(kr)}{k} - a \cos(kr)g(r) \quad (\text{A10})$$

and $g(r) \rightarrow 1$ for $r \geq R$. The first integral can be evaluated after dropping the pure Coulomb piece. We find

$$\begin{aligned} \int_R^\infty \phi^2(r) \frac{dr}{r} &= a \text{si}(2kR) - a^2 \text{Ci}(2kR) \\ &\cong -\frac{\pi a}{2} + 2kRa - a^2[\gamma + \ln(2kR)], \end{aligned} \quad (\text{A11})$$

where we have expanded the sine and cosine integrals for small k . Using Eqs. (A5)–(A8) and substituting (A9) into $k \cot \delta_0^c$ in Eq. (A5), we find that

$$\frac{1}{a_C} \cong \frac{1}{a} + \Delta + \xi[2\gamma + \ln(\xi)], \quad (\text{A12})$$

where

$$\Delta = \frac{2\xi}{a} \int_0^\infty [g(r) - 1] dr - \xi \int_0^R dr \frac{g^2(r)}{r} + \xi \ln R. \quad (\text{A13})$$

The expression (A13) is independent of R for sufficiently large R , and is now independent of the diverging factors of $1/k$ and $\ln(k)$. This expression is our primary result in this appendix. We note that the $\ln(\xi)$ term arose from $\ln(\xi)$ in Eq. (A8). Comparing with Eq. (A1) we find

$$\epsilon = -\frac{2}{a} \int_0^\infty [1 - g(r)] dr - \int_0^R dr \frac{g^2(r)}{r} + \ln R, \quad (\text{A14})$$

$$\lambda - 1 = -2\xi \int_0^\infty [1 - g(r)] dr, \quad (\text{A15})$$

and

$$\delta = \xi[\ln(\xi) + 2\gamma] - \xi \int_0^R dr \frac{g^2(r)}{r} + \xi \ln(R). \quad (\text{A16})$$

Note that the condition $\lambda < 1$ corresponds to $\int_0^\infty (1 - g) dr > 0$. Since $g(r)$ vanishes at $r = 0$ and asymp-

totically approaches 1, this will occur in most circumstances.

For the Yamaguchi model it is easily found that

$$\Delta = -\frac{2\xi}{\alpha\beta} - \xi[\gamma + \ln(\beta/2)], \quad (\text{A17})$$

which agrees with the perturbative expansion of the exact result. This confirms the correctness of our expressions. The various expansions we have made are correct but the procedure lacks rigor; doubtless they can be made mathematically respectable.

For the three-body problem we must integrate Eq. (A13) over the Jacobi coordinates \vec{x} and \vec{y} , instead of just r , which corresponds to y . This is a trivial change, and is easily implemented.

We can also make a connection between (A14) and the standard expression for the effective range, r_0 ,

$$\frac{r_0}{2} = \frac{-2}{a} \int_0^\infty r(1-g)dr - \int_0^\infty (g^2-1)dr. \quad (\text{A18})$$

Except for a factor of $1/r$ in each integrand, Eq. (A14) is the same as Eq. (A18). Physically, this is reasonable and reminds us that the "effective range" determines the amount of the Coulomb energy shift. The precise amount depends on the balance of the two contributions, which is sensitive to the size of a .

Finally, anyone interested in the extension of Coulomb scattering lengths and effective ranges to nonzero l should consult Ref. 33.

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