

Convergence of Faddeev partial-wave series for triton ground state

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An iterative technique was used to solve the Faddeev equations, which determine the bound state of the triton, for the Reid soft core, Argonne v_{14} , super soft core (C), and de Tourreil-Rouben-Sprung (B) potential models. Separate solutions for each model were generated for 5, 9, 18, 26, and 34 three-body channels, the latter corresponding to all two-nucleon partial waves with $J \leq 4$. The results indicate that the odd partial waves do not contribute substantially to the energy, and that the $J > 4$ partial waves probably contribute less than 10 keV. Coulomb energies, radii, and probability percentages of various wave function components were also calculated.

I. INTRODUCTION

Many techniques have been used to solve the Schrödinger equation for three nucleons. The august Rayleigh-Ritz variational method was the first technique applied to "realistic" potentials,¹ which include the complexities of spin and isospin as well as a strong tensor force. The additional complication of a strong short-range repulsion between two nucleons substantially slows the convergence of the variational upper bound to the exact eigenvalue as the trial wave function becomes exact. Modern applications also have some difficulty handling the strong tensor force.²

Other methods are not free of this problem, and, indeed, introduce new ones. Various discretization procedures map the original "exact" Schrödinger equation into a truncated problem which can be solved exactly in a numerical sense. In the hyperspherical technique³ one expands the wave function as an infinite series of generalized partial waves, obtaining a finite set of coupled ordinary differential equations to be solved after truncating the series. Conversely, in the Faddeev method⁴ one expands the (local) two-nucleon potential as a sum of nonlocal potentials, each of which acts in a single two-nucleon partial wave, a problem that can be solved exactly in the numerical sense. The Green's function Monte Carlo method,⁵ which holds great promise for nuclear physics, has not yet been applied quantitatively to this problem because of difficulties with fermion degrees of freedom. Brute force attempts to solve the Schrödinger equation directly⁶ have not proven particularly successful.

The Tower of Babel situation with disparate approximations has been distracting, since no benchmark solutions exist for physically realistic problems. Accurate calculations are also necessary if one wishes to assess the importance of three-body forces, since first-order perturbation theory may not be adequate. In this study we present calculations within the Faddeev framework, which include up to 34 three-nucleon partial waves, and variational upper bounds based on these wave functions. The Fad-

deev partial-wave series converges rapidly. For our largest calculations, possibly the largest ever attempted, we believe that the binding energy is converged to within 10 keV of the solution for the complete Schrödinger problem, and therefore provides a benchmark for other calculational techniques. An interesting subsidiary result is that the odd nucleon-nucleon partial waves contribute minimally to the trinucleon binding energy.

Traditionally, Faddeev calculations are categorized by numbers of channels, with each channel specifying the angular momentum quantum numbers of an interacting pair of nucleons, and the corresponding quantum numbers of the remaining spectator nucleon with respect to the center of mass of the pair.⁷ There are, therefore, two such channels for each nucleon-nucleon partial wave, except for total two-nucleon angular momentum J equal to zero, which is restricted to one. Typically, one solves for 5 or 18 channels, the former including only the ($^1S_0, ^3S_1-^3D_1$) pair partial waves (all even parity waves with $J \leq 1$) and the latter including all pair partial waves with $J \leq 2$. We report in Sec. III calculations corresponding to 9 channels (even waves only for $J \leq 2$), 26 channels ($J \leq 4$ with no odd waves for $J=3$ and 4), and 34 channels (all waves with $J \leq 4$), as well as the standard 5 and 18 channel calculations. These solutions were obtained for the Reid soft core,⁸ Argonne v_{14} ,⁹ super soft core (C),¹⁰ and de Tourreil-Rouben-Sprung (B) (Ref. 11) potential models.

Our best results have a defect of 0.8–1.1 MeV in the theoretical binding energies of ^3H compared with the experimental value. This may indicate the presence of a significant contribution from three-nucleon forces. We also demonstrate that perturbation theory for the $J \leq 2$ odd partial waves is not particularly successful.

II. NUMERICAL METHODS

Following the procedures used in our previous configuration-space Faddeev calculations,⁷ we write the total wave function for three identical nucleons as the sum of the three Faddeev amplitudes:

$$\begin{aligned}\Psi &= \psi(\mathbf{x}_1, \mathbf{y}_1) + \psi(\mathbf{x}_2, \mathbf{y}_2) + \psi(\mathbf{x}_3, \mathbf{y}_3), \\ &\equiv \psi_1 + \psi_2 + \psi_3,\end{aligned}\quad (1)$$

where we use the Jacobi variables

$$\mathbf{x}_i = \mathbf{r}_j - \mathbf{r}_k \quad (2a)$$

and

$$\mathbf{y}_i = \frac{1}{2}(\mathbf{r}_j + \mathbf{r}_k) - \mathbf{r}_i. \quad (2b)$$

The Schrödinger equation can be separated into three coupled Faddeev equations:

$$[T + V(\mathbf{x}_i) - E]\psi_i = -V(\mathbf{x}_i)(\psi_j + \psi_k). \quad (3)$$

For identical particles the Faddeev amplitudes ψ_i all have the same functional form, and it is only necessary to solve one of these Faddeev equations. We use the j - J coupling scheme for the partial wave representation of the Faddeev amplitudes and write ψ_i in the form:

$$\psi(\mathbf{x}_i, \mathbf{y}_i) = \sum_{\alpha} \frac{\psi_{\alpha}(\mathbf{x}_i, \mathbf{y}_i)}{x_i y_i} |[(l_{\alpha}, s_{\alpha})j_{\alpha}; (L_{\alpha}, S_{\alpha})J_{\alpha}]\mathcal{F}M; (t_{\alpha}T_{\alpha})\mathcal{T}M_{\mathcal{T}}\rangle_i, \quad (4)$$

where l_{α} is the relative orbital angular momentum of particles j and k ; s_{α} is the spin angular momentum of particles j and k ; j_{α} is the total angular momentum of particles j and k ; L_{α} is the orbital angular momentum of particle i relative to the center of mass of particles j and k ; S_{α} is the spin of particle i ($S_{\alpha} = \frac{1}{2}$); J_{α} is the total angular momentum of particle i ; \mathcal{F} is the total angular momentum of the three-body system; t_{α} is the total isospin of particles j and k ; T_{α} is the isospin of particle i ($T_{\alpha} = \frac{1}{2}$); \mathcal{T} is the total isospin of the three-body system.

Following Noyes¹² we introduce the hyperspherical variables defined by

$$x_i = \rho \cos\theta \quad (5a)$$

and

$$y_i = \frac{1}{2}\sqrt{3}\rho \sin\theta. \quad (5b)$$

Now the Faddeev equation for ψ_{α} can be written in the form

$$\begin{aligned}\left[\frac{\partial^2}{\partial \rho^2} + \frac{1}{\rho} \frac{\partial}{\partial \rho} + \frac{1}{\rho^2} \frac{\partial^2}{\partial \theta^2} - \frac{l_{\alpha}(l_{\alpha}+1)}{\rho^2 \cos^2 \theta} - \frac{L_{\alpha}(L_{\alpha}+1)}{\rho^2 \sin^2 \theta} - \kappa^2 \right] \psi_{\alpha}(\rho, \theta) - \sum_{\beta} v_{\alpha\beta}(\rho \cos\theta) \psi_{\beta}(\rho, \theta) \\ = \sum_{\beta\gamma} v_{\alpha\gamma}(\rho \cos\theta) \int_{\theta^-}^{\theta^+} K_{\gamma\beta}(\theta, \theta') \psi_{\beta}(\rho, \theta') d\theta', \quad (6)\end{aligned}$$

where $\kappa^2 = -mE/\hbar^2$ and $v_{\alpha\beta}(\rho \cos\theta)$ is m/\hbar^2 times the partial wave projection of $V(\mathbf{x}_i)$. The $K_{\gamma\beta}(\theta, \theta')$ can be evaluated by standard angular momentum recoupling techniques,¹³ and θ^+ and θ^- are defined in Ref. 7.

The numerical calculations are facilitated by defining a smoother function $F_{\alpha}(\rho, \theta)$ by

$$\psi_{\alpha}(\rho, \theta) = F_{\alpha}(\rho, \theta) \frac{e^{-\kappa\rho}}{\rho^{1/2}}.$$

Equation (6) then has the form

$$\begin{aligned}\left[\frac{\partial^2}{\partial \rho^2} + \frac{1}{4\rho^2} + \frac{1}{\rho^2} \frac{\partial^2}{\partial \theta^2} - 2\kappa \frac{\partial}{\partial \rho} - \frac{l_{\alpha}(l_{\alpha}+1)}{\rho^2 \cos^2 \theta} - \frac{L_{\alpha}(L_{\alpha}+1)}{\rho^2 \sin^2 \theta} \right] F_{\alpha}(\rho, \theta) - \sum_{\beta} v_{\alpha\beta}(\rho \cos\theta) F_{\beta}(\rho, \theta) \\ = \sum_{\beta\gamma} v_{\alpha\gamma}(\rho \cos\theta) \int_{\theta^-}^{\theta^+} K_{\gamma\beta}(\theta, \theta') F_{\beta}(\rho, \theta') d\theta', \quad (7)\end{aligned}$$

with the boundary conditions

$$F_{\alpha}(\rho, \theta) = 0 \text{ for } \rho = 0, \quad (8a)$$

$$F_{\alpha}(\rho, \theta) = 0 \text{ for } \theta = 0 \text{ and } \pi/2, \quad (8b)$$

$$\frac{\partial F_{\alpha}(\rho, \theta)}{\partial \rho} = 0 \text{ for } \rho = \rho_{\max}. \quad (8c)$$

To solve Eq. (7) we use the orthogonal collocation technique.¹⁴ First the $F_\alpha(\rho, \theta)$ are expanded in bicubic Hermite splines on a rectangular grid in the ρ - θ coordinates:

$$F_\alpha(\rho, \theta) = \sum_{m=1}^M \sum_{n=1}^N a_{mn}^\alpha s_m(\rho) s_n(\theta). \quad (9)$$

The orthogonal collocation procedure requires that one determine the values of a_{mn}^α for which the functions $F_\alpha(\rho, \theta)$ satisfy Eq. (7) at M distinct values of ρ_i and N distinct values of θ_j (the orthogonal collocation points). Thus we require that

$$\begin{aligned} \sum_{m=1}^M \sum_{n=1}^N \left\{ s_m''(\rho_i) s_n(\theta_j) + \frac{1}{\rho_i^2} \left[\frac{1}{4} - \frac{l_\alpha(l_\alpha+1)}{\cos^2 \theta_j} - \frac{L_\alpha(L_\alpha+1)}{\sin^2 \theta_j} \right] s_m(\rho_i) s_n(\theta_j) + \frac{1}{\rho_i^2} s_m(\rho_i) s_n''(\theta_j) \right. \\ \left. - 2\kappa s_m'(\rho_i) s_n(\theta_j) \right\} a_{mn}^\alpha - \sum_{m=1}^M \sum_{n=1}^N \sum_{\beta} [v_{\alpha\beta}(\rho_i \cos \theta_j) s_m(\rho_i) s_n(\theta_j)] a_{mn}^\beta \\ = \sum_{m=1}^M \sum_{n=1}^N \sum_{\beta} \left\{ \sum_{\gamma} v_{\alpha\gamma}(\rho_i \cos \theta_j) \left[\int_{\theta_j^-}^{\theta_j^+} K_{\gamma\beta}(\theta_j, \theta') s_n(\theta') d\theta' \right] s_m(\rho_i) \right\} a_{mn}^\beta. \quad (10) \end{aligned}$$

In our previous calculations⁷ we wrote this equation as a matrix eigenvalue problem for κ and then used the power technique¹⁵ to solve for κ and the a_{mn}^α . This requires the solution of very large matrix equations and the numerical calculations become prohibitive for more than five channels. Consequently, for our present calculations we adopt a different technique. Equation (10) is of the form

$$\sum_{\beta} \sum_m \sum_n A_{\alpha ij, \beta mn} a_{mn}^\beta = \sum_{\beta} \sum_m \sum_n B_{\alpha ij, \beta mn} a_{mn}^\beta \quad (11)$$

which can be written as the matrix equation

$$Aa = Ba. \quad (12)$$

However, the $A_{\alpha ij, \beta mn}$ depend parametrically upon the unknown κ . In order to solve the equation we introduce a new parameter λ and rewrite Eq. (12) in the form

$$Aa = \lambda Ba. \quad (13)$$

For a fixed value of κ , this becomes a generalized eigenvalue problem with eigenvalue λ . Thus, to find the bound state energy we search for the value of κ for which the eigenvalue λ has the value unity. The advantage of using Eq. (13) is that the matrix A can be written in a block diagonal form. From Eq. (10) one can see that the only term which couples the different channels on the left-hand side is the $v_{\alpha\beta}$ term. Since the tensor force couples at most two channels, the inverse of A can be calculated for either one or two channels at a time depending on whether a tensor force is present or not. This considerably reduces both the computer time and memory requirements of the numerical algorithm described below.

Equation (13) can be solved by a variation of the power method. Because the power method yields the largest eigenvalue, we first rewrite the equation in the form

$$A^{-1}Ba = \frac{1}{\lambda} a. \quad (14)$$

Thus we now have a standard eigenvalue problem of the form

$$Ha = \Lambda a. \quad (15)$$

To solve this by the power method we assume an initial eigenvector $a^{(0)}$ and generate the sequence $a^{(n)}$, where

$$a^{(n)} = Ha^{(n-1)}. \quad (16)$$

This sequence will converge to the eigenvector with the largest (magnitude) eigenvalue Λ . However, it has been shown¹⁶ that for realistic potentials there may exist a negative eigenvalue λ whose absolute value is less than unity. Since we want to find the eigenvalue $\Lambda = 1/\lambda = 1.0$ as the largest eigenvalue of H , we cannot use the sequence generated by Eq. (16) in that case. In order to generate a sequence which does converge to the desired eigenvalue, we shift the spectrum of H ; i.e., we rewrite Eq. (15) in the form

$$(H + \sigma I)a = (\Lambda + \sigma)a. \quad (17)$$

With the proper choice of σ , the sequence

$$a^{(n)} = (H + \sigma I)a^{(n-1)} \quad (18)$$

will converge to the eigenvector corresponding to $\Lambda = 1.0$, when we choose the correct value for κ .

The actual numerical calculations were performed by first solving the equation

$$b^{(n)} = Ha^{(n-1)}, \quad (19)$$

which can be rewritten ($H = A^{-1}B$) in the form

$$Ab^{(n)} = Ba^{(n-1)}. \quad (20)$$

After solving Eq. (20) for $b^{(n)}$, one can use

$$a^{(n)} = b^{(n)} + \sigma a^{(n-1)} \quad (21)$$

to find the next vector in the sequence. This algorithm is identical in practice to solving Eq. (16) rewritten as

$$a^{(n)} = Ha^{(n-1)}, \quad (22)$$

and then using

$$\tilde{a}^{(n)} = a^{(n)} + \sigma \tilde{a}^{(n-1)}. \quad (23)$$

This procedure is similar to the averaging of eigenvector iterates used previously¹⁷ to eliminate undesired oscillations in the sequence generated by the power method when a matrix has positive and negative eigenvalues with approximately the same absolute value.

III. RESULTS AND CONCLUSIONS

For each of the four potentials listed in the Introduction, Reid soft core (RSC), Argonne v_{14} (AV14), super soft core (SSC) (C), and de Tournell-Rouben-Sprung (TRS) (B), the Faddeev equations were solved retaining 5, 9, 18, 26, and 34 channels. For purposes of comparison with previous results, RSC and AV14 results were also obtained for three channels (*s*-wave spectator with 1S_0 , 3S_1 - 3D_1 forces). We note that our SSC (C) potential, generously provided by Sprung, has slightly different singlet-odd forces than the published version. These partial waves typically contribute *in toto* less than 20 keV of the binding, and only 12 keV for the SSC (C) potential, so the difference is quite negligible. The RSC partial-wave potentials for $J > 2$ were taken from Day.⁸

Two different sets of meshes were used.⁷ For the smaller number of channels we used 20 break points in both ρ and θ , extending to 24 fm in ρ , scaled by 1.3, and using a (12,5,3) distribution in θ . The ρ scaling means that the break points were not equally spaced:

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

The θ splines were distributed uniformly in each of three equally spaced intervals between 0 and $\pi/2$; the interval nearest $\pi/2$, where the two-body potential is largest, contained the most splines. For the large number of channels we reduced the number of splines to 14, the maximum value of ρ being 20 fm, and the θ distribution being (9,3,2). As stated earlier, we solved for a strength parameter λ , rather than the eigenenergy κ^2 , and extrapolated to $\lambda=1$. We subsequently found that in the vicinity of $\lambda=1.0$, a small change of $\Delta\lambda=10^{-4}$ corresponded to a change of approximately 1.7 keV in the binding energy, E_B . Results were checked using the Rayleigh-Ritz¹⁸ variational procedure. In addition to calculating $\langle H \rangle$, we have also calculated the point Coulomb energy, E_C^0 , the Coulomb energy, E_C (corresponding to a dipole nucleon form factor), the hyperspherical approximation to E_C , E_C^H , the point nucleon rms charge radii, $\langle r^2 \rangle_{\text{He}}^{1/2}$ and $\langle r^2 \rangle_{\text{H}}^{1/2}$ (for ^3He and ^3H , respectively), and the probability percentage of S' , P , and D states. These results are shown in Table I. We have also calculated, but not tabulated, the percentage of S'' state, which arises solely from the odd-parity nucleon-nucleon partial waves; typically, this number is of order $3-5 \times 10^{-5}$, except for the RSC potential, where the value of 2×10^{-4} reflects the unusual p waves of that potential. The P -state percentage can be further

TABLE I. Results of trinucleon Faddeev calculations for 3, 5, 9, 18, 26, and 34 channels for four different potential models, as well as calculated Coulomb energies, charge radii, and percentages of S' , P , and D states.

Model		E_B (MeV)	$-\langle H \rangle$ (MeV)	E_C^0 (keV)	E_C (keV)	E_C^H (keV)	$\langle r^2 \rangle_{\text{He}}^{1/2}$ (fm)	$\langle r^2 \rangle_{\text{H}}^{1/2}$ (fm)	$P_{S'}$ (%)	P_P (%)	P_D (%)
RSC	3 ^a	6.384	6.385	613	589	597	1.99	1.77	1.91	0	8.01
	5 ^a	7.023	7.023	635	609	616	1.89	1.70	1.67	0.08	9.34
	9 ^a	7.210	7.211	642	615	622	1.87	1.68	1.60	0.09	9.43
	18 ^a	7.231	7.231	643	616	624	1.87	1.68	1.46	0.08	9.42
	18	7.225	7.225	647	620	628	1.86	1.68	1.44	0.08	9.43
	26	7.342	7.342	647	620	628	1.85	1.67	1.41	0.08	9.50
	34	7.346	7.345	648	620	628	1.85	1.67	1.40	0.08	9.50
AV14	3	6.803	6.803	628	601	609	1.94	1.75	1.53	0	7.55
	5 ^a	7.441	7.441	647	619	626	1.86	1.68	1.36	0.08	8.86
	9 ^a	7.569	7.569	651	623	630	1.84	1.67	1.32	0.08	8.91
	18 ^a	7.573	7.573	653	624	632	1.84	1.67	1.14	0.08	8.90
	26	7.667	7.667	656	627	634	1.83	1.67	1.12	0.08	8.96
	34	7.670	7.669	656	627	634	1.83	1.67	1.12	0.08	8.96
SSC (C)	5 ^a	7.457	7.457	653	620	626	1.86	1.68	1.40	0.06	7.96
	9 ^a	7.521	7.521	654	622	628	1.85	1.68	1.38	0.06	8.00
	18 ^a	7.490	7.490	654	622	628	1.85	1.69	1.25	0.06	7.95
	18	7.490	7.490	654	622	628	1.85	1.68	1.25	0.06	7.95
	26	7.535	7.535	655	623	629	1.85	1.68	1.24	0.06	7.98
	34	7.534	7.534	655	623	629	1.85	1.68	1.24	0.06	7.98
TRS (B)	5 ^a	7.470	7.431	654	622	628	1.85	1.67	1.52	0.06	8.57
	5	7.493	7.443	654	621	628	1.85	1.67	1.53	0.06	8.57
	9	7.555		655	623	630	1.85	1.66	1.51	0.06	8.60
	18	7.516		656	623	630	1.85	1.67	1.34	0.06	8.56
	26	7.569		657	624	631	1.84	1.67	1.32	0.06	8.60
	34	7.565		657	624	631	1.84	1.67	1.32	0.06	8.60

^aCalculated with 20 ρ and θ break points.

broken down into that for the 4P and three separate 2P states (P, P', P'') if desired.

Our triton binding energies compare favorably with several recent Faddeev calculations. Five-channel calculations for the RSC potential by Bömelburg¹⁹ yielded -7.04 MeV, by Ishikawa *et al.*²⁰ yielded -7.03 MeV, and by Hajduk and Sauer¹⁶ yielded -7.023 MeV. The large 18 channel calculations by Ishikawa *et al.* gave -7.24 MeV and those of Hajduk and Sauer yielded -7.232 MeV. Chauvin *et al.*²¹ found -7.50 and -7.51 MeV for the five channel SSC (C) and TRS (B) potentials. Variational calculations have typically yielded upper bounds of $-6.7 \rightarrow -7.0$ MeV and extrapolate to a larger binding energy.

All of our results can be qualitatively understood in simple terms. The Coulomb energies scale roughly as $1/\langle r^2 \rangle^{1/2}$; more precisely²² they scale as $\langle 1/r \rangle$, which is the hyperspherical approximation to the Coulomb energy. The latter is between 1% and 1.5% too high, which nevertheless is an excellent approximation. The difference of the ${}^3\text{He}$ and ${}^3\text{H}$ charge radii reflects the difference between the nn and np forces; the former is the weaker and allows the two like nucleons to be further from the center of mass than the odd nucleon. Thus the charge radius of ${}^3\text{He}$ is larger than the mass radius, while the converse holds for ${}^3\text{H}$. The difference varies from 0.17 to 0.22 fm for the potential models studied. The radii decrease with increasing binding²³ roughly as $E_B^{-1/2}$, if the wave function tails dominate. The percentage of S' state, P_S , roughly reflects the difference of np and nn forces. It decreases as the number of channels increases (i.e., the force becomes more complete). This decrease may simply reflect the stiffening of the "effective spring constant" as the binding increases, thereby leading to a decrease in the size of the S' state, which is but a mixture of excited states in a shell-model description. The trinucleon P states arise only from a subset of the non- s waves for both interacting pair and spectator, which typically contribute only 2–3% of the potential energy; their percentage is correspondingly miniscule. The complete D -state percentage for each case is very close (within 3%) to 1.5 times the corresponding D -state percentage of the deuteron. This result can be understood approximately if one performs a perturbation theory analysis,²⁴ as is demonstrated in the Appendix. The higher partial waves (beyond 3S_1 - 3D_1) generate small tensor force contributions.

Table II breaks down the contributions to $\langle H \rangle$ for the RSC 34 channel case into kinetic energy, $\langle T \rangle$, and potential energy, $\langle V \rangle$, while the latter is further decomposed according the nucleon-nucleon (partial wave) total angular momentum and parity. The bulk of the binding arises from the 3S_1 - 3D_1 ($J^\pi=1^+$) component of the force. The higher partial waves ($J=2, 3$, and 4) are much smaller and decrease rapidly in importance because of the angular momentum barrier. We believe the contribution to the binding energy of partial waves with $J>4$ to be only a few keV. Also of interest is the very small contribution of negative parity waves (-0.2 MeV) in going from 9 channels (positive parity $J \leq 2$) to 18 channels (all $J \leq 2$). In each case in Table I, the transition from 9 to 18 channels, or 26 to 34 channels involves minimal accrual of binding.

TABLE II. Decomposition of the RSC 34 channel binding energy into kinetic and potential energy parts, and the further breakdown of the latter by nucleon-nucleon (partial-wave) total angular momentum and parity. All energies are in MeV.

	$\langle V_J^{(p)} \rangle$	$\langle V_J \rangle$	$\langle V^{(p)} \rangle$
0^+ :	-13.553		
0^- :	-0.176		
0:		-13.729	
1^+ :	-43.874		
1^- :	+0.227		
1:		-43.647	
2^+ :	-0.188		
2^- :	-0.247		
2:		-0.435	
3^+ :	-0.117		
3^- :	+0.002		
3:		-0.115	
4^+ :	-0.014		
4^- :	-0.006		
4:		-0.020	
(+):			-57.746
(-):			-0.200
Total $\langle V \rangle$:			-57.946
$\langle T \rangle$:			+50.600
$\langle H \rangle$:			-7.345

The last figure quoted for the various energies presented in Tables I and II is not necessarily significant. We have chosen to quote at the keV level so that differences of energies can be easily assessed. The latter should be reliable under variation of quadrature meshes, even though the minuend or subtrahend is not.

The results for the TRS (B) potential are only partially complete. The variational bounds are rather considerably at variance (~ 50 keV) with the Faddeev eigenvalues. We have traced at least part of the problem to the unusual structure of this potential, which is very smooth for small distances but then abruptly changes. This change in the region from 0.5 to 1.0 fm necessitates a rather severe redistribution of spline break points. The scaling algorithm that we have used was designed to handle the strong short-range repulsion, and not abrupt midrange variations. Nevertheless, because our results are reasonably satisfactory (though less so than for the other potentials), because we are interested primarily in convergence with respect to J , and because the TRS (B) potential is quite similar to SSC (C), we have chosen not to redesign our spline mesh to accommodate this particular model.

Finally, we address the question of whether the effect of the higher-order partial waves can be determined accurately using first-order perturbation theory. In Ref. 22 we developed a simple trick to decompose the Coulomb energy into first- and second-order contributions (in α , the fine structure constant), assuming that third order is negligible. This technique has been extended²⁵ by Hajduk to the next order. Writing a Hamiltonian H as $H_0 + \Delta H$, where ΔH is a (presumably) small perturbation and where $H|\Psi\rangle = E|\Psi\rangle$ and $H_0|\Psi_0\rangle = E_0|\Psi_0\rangle$, we can calculate four independent quantities, in addition to

TABLE III. Decomposition of RSC binding differences (by channel) according to their perturbation theory content using Hajduk's relations. Here, the E_i represent powers of λ , where $\lambda\Delta H$ is the difference of the Hamiltonians for n and m channels. All energies are in MeV.

Channels	E	E_0	E_1	E_2	E_3
5-9	-7.210	-7.023	-0.174	-0.014	0.001
9-18	-7.231	-7.210	+0.511	-0.891	0.359
18-26	-7.342	-7.225	-0.099	-0.020	0.003
26-34	-7.345	-7.342	-0.003	0.0001	-0.0003

$$\langle \Psi | H | \Psi \rangle \equiv E:$$

$$\langle \Psi_0 | H_0 | \Psi_0 \rangle \equiv E_0, \quad (24)$$

$$\langle \Psi_0 | \Delta H | \Psi_0 \rangle \equiv E_1, \quad (25)$$

$$\langle \Psi | \Delta H | \Psi \rangle \equiv \overline{\Delta E}, \quad (26)$$

$$\langle \Psi | H_0 | \Psi \rangle \equiv \overline{E}_0. \quad (27)$$

Further assuming that E_4 , the contribution to E from fourth order in ΔH , is negligible, we can use the standard perturbation theory expressions²⁴ and solve for E_2 and E_3 , in addition to the trivially obtained E_0 and E_1 . Hajduk's relations are

$$E = E_0 + E_1 + E_2 + E_3, \quad (28)$$

$$E_0 = \langle \Psi_0 | H_0 | \Psi_0 \rangle, \quad (29)$$

$$E_1 = \langle \Psi_0 | \Delta H | \Psi_0 \rangle, \quad (30)$$

$$E_2 = 2\overline{\Delta E} + 3\overline{E}_0 - 3E_0 - 2E_1 = 3(E - E_0) - 2E_1 - \overline{\Delta E}, \quad (31)$$

$$E_3 = -\overline{\Delta E} - 2\overline{E}_0 + 2E_0 + E_1 = -2(E - E_0) + E_1 + \overline{\Delta E}. \quad (32)$$

We apply these relations to the RSC potential and the 5-9, 9-18, 18-26, and 26-34 channel eigenvalue differences, which are given in Table III. As an example, the necessary energies for the 5-9 channel differences are $E - E_0 = -0.1873$, $E_1 = -0.1737$, and $\overline{\Delta E} = -0.2004$, leading to the results shown in the first line of Table III. This 5-9 channel energy difference is accurately given by perturbation theory; conversely, the 9-18 channel difference is not even closely approximated by first-order perturbation theory.²⁶ The reason is that the odd nucleon-nucleon partial waves couple strongly to the *small* components of the wave function which are substantially modified, as evinced by Table I. Large fractional changes in these components couple back to the potential and produce large second-order (and higher) energy shifts. In fact the 5-18 channel shift in perturbation theory is roughly 260 keV *repulsive*, while the complete result is roughly 210 keV *attractive*. The positive parity 18-26 channel shift and the negative parity 26-34 channel shift are dominated by the first-order result. Qualitatively similar conclusions hold for the other potentials. This result appears to contradict the results of Ref. 27.

IV. SUMMARY

In conclusion, we have calculated Faddeev eigenvalues and variational bounds, Coulomb energies, radii, and component probability percentages of states for 5, 9, 18, 26, and 34 channel approximations in the solution of the triton ground state for four different potential models. Variational bounds and Faddeev eigenvalues are in excellent agreement, except for the slightly less satisfactory TRS (B) potential results. Convergence with increasing J is evident and we estimate less than 10 keV for the omitted $J > 4$ higher partial waves. Negative parity nucleon-nucleon partial waves play only a small role in the binding energies, although they modify the small wave function components (S' and P states) non-negligibly. A perturbation theory analysis indicates that first-order perturbation theory works quite well for the positive parity nucleon-nucleon partial waves, but not at all for the $J \leq 2$ negative parity waves. Coulomb energies and radii vary predictably with binding energy; the S' -state probability generally decreases with increasing binding energy (although not universally), while the D -state probability seems determined by the corresponding probability for the deuteron.

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APPENDIX: D -STATE PROBABILITY RELATIONS

In order to relate the D -state probability percentage for deuteron (d), triton (t), and alpha (α) particles, we make six specific assumptions. Although the accuracy of these *Ansätze* is difficult to access, they are all reasonable. We also note that calculating percentages of various wave function components is a theorist's game; it is possible to prove using general arguments²⁸ that such quantities are not measurable. They are nevertheless useful theoretical constructs.

We assume that (1) perturbation theory can reproduce the D state of each system; (2) we can neglect mixed symmetry S states and all P states, leaving only spatially symmetric S states as our basis; (3) high-momentum com-

ponents dominate the tensor force, and create virtual states of high energy; (4) the energy of these virtual states is roughly independent of system; (5) in the t and α the three- and four-body contributions to P_D are negligible; (6) the correlation functions for the d , t , and α particles are the same.

Given our s -wave basis functions Ψ_0 , the D -wave component is given perturbatively by

$$\Psi_D = G'(E_0) V_T \Psi_0 \equiv \sum_{N \neq 0} \frac{|N\rangle \langle N | V_T | \Psi_0 \rangle}{E_0 - E_N} \quad (\text{A1})$$

and

$$P_D = \sum_{N \neq 0} \frac{\langle 0 | V_T | N \rangle \langle N | V_T | 0 \rangle}{(E_0 - E_N)^2}, \quad (\text{A2})$$

where V_T is the tensor potential. Following Riska and Brown,²⁹ Hadjimichael, Yang, and Brown,³⁰ and Jackson and Riska,³¹ we approximate $E_N - E_0$ by \bar{E} , use the closure approximation, and write

$$P_D \cong \langle 0 | V_T^2 | 0 \rangle / \bar{E}^2. \quad (\text{A3})$$

The quasideuteron approximation, assessed in Refs. 29–31, presumes that \bar{E} is large and thus independent of the system, because only the interacting two-body pair is important. Moreover, since V_T is a two-body operator, V_T^2 generates two-, three-, and four-body terms. Because of the high momentum components involved, which are lacking in Ψ_0 , the three- and four-body terms should be considerably suppressed. Because our basis is space symmetric, we can factor the spin-isospin function from the matrix element in Eq. (A3):

$$P_D \sim \lambda_A (\langle 0 | V_T^0 | 0 \rangle / \bar{E}^2), \quad (\text{A4})$$

where V_T^0 is the radial part of the two-body tensor force, and λ_A is the spin-isospin matrix element for $A=2,3,4$. Performing this latter algebra we find that all P_D 's are simply proportional if the radial matrix elements and \bar{E} (term in parentheses above) are independent of A . In particular, we obtain

$$P(D) = \frac{3}{2} P_D \text{ (triton)} \quad (\text{A5})$$

and

$$P(D) = 3P_D \text{ (}\alpha \text{ particle)}, \quad (\text{A6})$$

where P_D is the deuteron D -state percentage.

The key ingredient is the use of perturbation theory based on a symmetric spatial state. This corresponds to s -wave pairs and since the tensor operator S_{12} annihilates spin-singlet pairs, the tensor-force interacting pairs have isospin zero ($T=0$). This guarantees that in the two-body parts of V_T^2 only the $T=0$ part contributes, rendering this independent of the detailed isospin structure of V_T itself. Moreover, the deuteron has one such triplet; the triton and α have three and six interacting pairs which are half triplet and half singlet. This gives directly the ratio 1:3/2:3. The other key ingredient is neglecting the three- and four-body terms and assuming that radial matrix elements (correlation functions) are identical. Within that framework the closure approximation is not actually necessary. We note that triton correlation functions look very much like the corresponding deuteron wave functions.²³

We have seen that $P(D)/P_D = 1.5$ is a very good approximation for local two-body potentials in the triton. The linear relationship appears to hold equally well for separable potentials, although for rank-one spin-triplet forces with no short-range repulsion the ratio is only 1.3.³² We note that Eq. (A5) was asserted without proof in Ref. 33.

In the α particle there is some theoretical evidence^{34,35} that $P(D)$ is 50–100% greater than $P(D)$ for the triton, although this has been contested by Goldhammer.³⁶ The experimental evidence for a D -wave component in the α particle centers on the asymptotic D -wave normalization, as it does in the triton. The ratio of the asymptotic D - and S -wave normalizations for the deuteron,³⁷ triton,³⁸ and α particle^{39–41} are given roughly by 0.027, 0.05, and 0.3–0.5, which reflects increasing binding and, presumably, an increasing D -wave component. We note that in the α particle there are two separate asymptotic normalizations, corresponding to pulling it apart as ${}^3\text{He} + n$, and as $d + d$. The former clearly has no D -wave asymptotic component, although it is the dominant part of the complete wave function. The deuteron and α -particle correlation functions are similar.⁴²

¹L. M. Delves, *Adv. Nucl. Phys.* **5**, 1 (1972) reviews this topic thoroughly.

²J. Lomnitz-Adler and V. R. Pandharipande, *Nucl. Phys.* **A342**, 404 (1980).

³J. L. Ballot and M. Fabre de la Ripelle, *Ann. Phys. (N.Y.)* **127**, 62 (1980).

⁴L. D. Faddeev, *Zh. Eksp. Teor. Fiz.* **39**, 1459 (1960) [*Sov. Phys.—JETP* **12**, 1014 (1961)].

⁵J. G. Zabolitsky and M. H. Kalos, *Nucl. Phys.* **A356**, 114 (1981).

⁶I. M. Bassett, B. R. E. Lederer, and G. C. Vorlicek, *Phys. Lett.* **51B**, 329 (1974); *J. Comput. Phys.* **22**, 34 (1976).

⁷G. L. Payne, J. L. Friar, B. F. Gibson, and I. R. Afnan, *Phys. Rev. C* **22**, 823 (1980).

⁸R. V. Reid, Jr., *Ann. Phys. (N.Y.)* **50**, 411 (1968); B. Day, *Phys. Rev. C* **24**, 1203 (1981).

⁹R. B. Wiringa, R. A. Smith, and T. A. Ainsworth, *Phys. Rev. C* **29**, 1207 (1984).

¹⁰R. de Tourreil and D. W. L. Sprung, *Nucl. Phys.* **A201**, 193 (1984).

¹¹R. de Tourreil, B. Rouben, and D. W. L. Sprung, *Nucl. Phys.* **A242**, 445 (1975).

¹²H. P. Noyes, in *Three Body Problems in Nuclear and Particle Physics*, edited by J. S. C. McKee and P. M. Rolph (North-Holland, Amsterdam, 1970), p. 2.

¹³E. P. Harper, Y. E. Kim, and A. Tubis, *Phys. Rev. C* **2**, 877 (1970); **6**, 126 (1972).

¹⁴P. M. Prenter, *Splines and Variational Methods* (Wiley, New

- York, 1975).
- ¹⁵G. Dahlquist and A. Bjorck, *Numerical Methods* (Prentice-Hall, Englewood Cliffs, 1977), p. 209.
- ¹⁶C. Hajduk and P. U. Sauer, Nucl. Phys. **A369**, 321 (1981).
- ¹⁷D. R. Lehman, private communication.
- ¹⁸J. L. Friar, B. F. Gibson, and G. L. Payne, Phys. Rev. C **24**, 2279 (1981).
- ¹⁹A. Bömelburg, Phys. Rev. C **28**, 403 (1983).
- ²⁰S. Ishikawa, T. Sasakawa, T. Sawada, and T. Ueda, Phys. Rev. Lett. **53**, 1877 (1984).
- ²¹J. Chauvin, C. Gignoux, J. J. Benayoun, and A. Laverne, Phys. Lett. **78B**, 5 (1978).
- ²²G. L. Payne, J. L. Friar, and B. F. Gibson, Phys. Rev. C **22**, 832 (1980).
- ²³J. L. Friar, B. F. Gibson, and G. L. Payne, Annu. Rev. Nucl. Part. Sci. **34**, 403 (1984).
- ²⁴L. I. Schiff, *Quantum Mechanics*, 3rd ed. (McGraw-Hill, New York, 1968).
- ²⁵C. Hajduk, private communication.
- ²⁶P. U. Sauer and C. Hajduk, private communication, in correspondence with us, first noticed this effect.
- ²⁷C. Gignoux and A. Laverne, Nucl. Phys. **A203**, 597 (1973) (see Table III).
- ²⁸J. L. Friar, Phys. Rev. C **20**, 325 (1979).
- ²⁹D. O. Riska and G. E. Brown, Phys. Lett. **32B**, 662 (1970).
- ³⁰E. Hadjimichael, S. N. Yang, and G. E. Brown, Phys. Lett. **39B**, 594 (1972).
- ³¹A. D. Jackson and D. O. Riska, Phys. Lett. **50B**, 207 (1974).
- ³²B. F. Gibson and D. R. Lehman, Phys. Rev. C **29**, 1017 (1984).
- ³³L. M. Delves, in *Few-Body Problems in Nuclear and Particle Physics*, edited by R. J. Slobodrian, B. Cujec, and K. Ramavartaram (Laval University, Quebec, 1975), p. 459.
- ³⁴Y. Akaishi, M. Sakai, J. Hiura, and H. Tanaka, Prog. Theor. Phys. **51**, 134 (1974); M. Sakai, I. Shimodaya, Y. Akaishi, J. Hiura, and H. Tanaka, *ibid.* **51**, 155 (1974); M. Wakamatsu, Nucl. Phys. **A329**, 381 (1979).
- ³⁵J. L. Ballot, Phys. Lett. **127B**, 399 (1983).
- ³⁶P. Goldhammer, Phys. Rev. C **29**, 1444 (1984).
- ³⁷J. L. Friar, B. F. Gibson, and G. L. Payne, Phys. Rev. C **30**, 1084 (1984).
- ³⁸J. L. Friar, B. F. Gibson, D. R. Lehman, and G. L. Payne, Phys. Rev. C **25**, 1616 (1982).
- ³⁹H. R. Weller, P. Colby, N. R. Roberson, and D. R. Tilley, Phys. Rev. Lett. **53**, 1325 (1984).
- ⁴⁰F. D. Santos, A. Arriaga, A. M. Eiro, and J. A. Tostevin, Phys. Rev. C **31**, 707 (1985).
- ⁴¹B. C. Karp, E. J. Ludwig, W. J. Thompson, and F. D. Santos, Phys. Rev. Lett. **53**, 1619 (1984).
- ⁴²M. Gari, H. Hebach, B. Sommer, and J. G. Zabolitsky, Phys. Rev. Lett. **41**, 1288 (1978).