Method for checking representations of three-nucleon Hamiltonians

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We describe a test for checking matrix elements of two-nucleon forces between three-nucleon wave functions by a comparison with matrix elements between two-nucleon wave functions. The test can be used to check both analytic and programming work. The test has been applied to a finite-difference representation of the triton Hamiltonian with the Hamada-Johnston potential using Derrick's matrix elements, and the analysis has been confirmed to high accuracy.

[NUCLEAR STRUCTURE Three-nucleon calculations; testing of matrix elements in analytic and numerical form.]

I. INTRODUCTION

Derrick and Blatt[1] show that the wave function for the ground state of the triton ($J^\pi = \frac{1}{2}^+$) with noncentral forces may be expressed, after elimination of the center-of-mass dependence, as a finite sum of terms:

$$\psi = \sum_{i=1}^{16} g_i(r_{12}, r_{23}, r_{13})\mathcal{Y}_i \qquad \text{(Euler angles, spin, isospin)}. \tag{1}$$

The three internucleon distances (r_{12}, r_{23}, r_{13}) specify the shape and size of the triangle formed by the three nucleons, and the Euler angles specify the orientation of this triangle in space. The 16 angle-spin-isospin functions $\mathcal{Y}_i$ have definite values for the orbital and spin angular momentum quantum numbers, for parity (even), and for the total isospin ($T = \frac{1}{2}$) and its z component ($T_z = \frac{1}{2}$). They also have definite permutation symmetry properties. The analytic forms for the $\mathcal{Y}_i$ are given in Ref. 1. The expansion (1) permits the reduction of the Schrödinger equation for the triton to an eigenvalue-eigenfunction problem of the form

$$H'g \equiv \rho \mathrm{H} g = \lambda \rho g . \tag{2}$$

In (2), H is a 16×16 matrix whose elements are the center-of-mass matrix elements of the triton Hamiltonian $\hat{H}$ between the functions $\mathcal{Y}_i$, ρ is a weight function, and g is a 16-component vector whose components are the g_i. The explicit matrix elements of $\hat{H}$ for the kinetic energy and for the usual terms occurring in modern nucleon-nucleon potentials are given by Derrick.[2,3] An individual matrix element of H may contain contributions from the kinetic energy operator and from all the terms of the potential energy, and so may contain functions and differential operators of first and second order in r_{12}, r_{23}, r_{13}. The contribution to H of each of the different terms of the potential (central, tensor, spin-orbit, and quadratic spin-orbit) consists in turn of a number of parts characterized by spin and parity (singlet or triplet, even or odd). If a function ϕ is expressible in the form (1) then we have, by the definition of H, and introducing the functions b_i,

$$\hat{H}\phi = \sum_i \left(\sum_j H_{ij} g_j \right) \mathcal{Y}_i \equiv \sum_i b_i(r_{12}, r_{23}, r_{13})\mathcal{Y}_i . \tag{3}$$

In Refs. 4 and 5, we have developed an approach to the solution of (2) which involves a direct finite-difference representation of H. The eigenvalue-eigenfunction problem is replaced by a series of eigenvalue-eigenvector problems defined on a series of diminishing mesh sizes. The complexity of H with the Hamada-Johnston potential, which we use, or with any of the "realistic" potentials, is such that in working with it, algebraic errors and errors of transcription are hard to avoid. To recheck Derrick's analytic work in obtaining H and to check our numerical representation and programming of it we have devised a searching test which may also be of use to other workers in the field of three-nucleon calculations.

The test is based on the following idea. Equation (3) allows us to obtain the action of the triton Hamiltonian (with c.m. dependence removed) on wave functions ϕ of form (1) by performing operations involving only the interparticle distances. If we can calculate independently

$$H^s\phi = (T + V_{12})\phi \tag{4}$$

(T is the three-particle kinetic energy in the c.m. system, V_{ij} is the potential energy between nucleons i and j), then H can be tested by setting V_{23} and V_{13} to zero in the expression for H, calculating $\hat{H}\phi$ using (3), and comparing the result with (4). This test will only be useful if (i) functions ϕ expressible in form (1) can be obtained which also allow $H^s\phi$ to be easily obtained analytically by a means independent of (3), and (ii) the comparison between $H^s\phi$ and (3) (with V_{23} and V_{13} equal to zero) can be easily made. If, further, H has been represented numerically, the numerical version of H may be used to calculate numerical estimates of $\hat{H}\phi$ via (3) and these may be compared with the analytic result $H^s\phi$. In this way the numerical representation and programming of H may be tested. While we have stated the test in terms of the particular case of expansion in the functions of Derrick and Blatt, it clearly may be generalized to any case where the Schrödinger equation for the three nucleons is reduced by expansion of the wave function in terms of special functions (for example, it could be used to test the matrix elements of the Cohen-Willis classification[12]). Both of the above requirements (i) and (ii) are met if ϕ is obtained by coupling two-nucleon wave functions and free-nucleon wave functions of definite angular momentum to give a three-nucleon wave function with $J=\frac{1}{2}$, $T=\frac{1}{2}$, and even parity. Since H^s is the sum of a two-nucleon Hamiltonian and a free-nucleon Hamiltonian, $H^s\phi$ is easily obtained analytically. By means of a series of recouplings of angular momenta Davies[6] has shown how such a ϕ may be expressed in the form (1), and with our choice for ϕ, this is also true for $H^s\phi$. Thus we have

$$H^s\phi = \sum_{i=1}^{16} c_i(r_{12}, r_{23}, r_{13})\mathcal{Y}_i .$$

Comparison of the easily calculable c_i with the b_i, when V_{13} and V_{23} have been set to zero in H, then checks H, since the $\mathcal{Y}_i$ are orthogonal. If the two-nucleon wave function is taken to have a certain spin and parity, the corresponding part of the potential is the only one contributing to Hg (i.e., to the b_i). By taking different spin-parity values for the two-nucleon wave function, all the contributions to H may be tested individually. By using permutation properties V_{23} and V_{13} may also be tested in the same way. Considerations somewhat similar to the above seem to have been used by Davies[7] to check analytic derivations of matrix elements but they have broader use in the testing of the numerical representation and programming of the analytic expressions, as we shall see in more detail in Sec. III.

In Sec. II we illustrate the method by showing how the triplet-odd contribution to the quadratic spin-orbit term may be tested. We also present explicit expressions for ϕ which can be used for testing the singlet-even and singlet-odd contributions, the results for the triplet-even having already been presented by Davies.[6] In Sec. III we show how a finite-difference version of H may be tested by numerically representing g, calculating the b_i on a series of mesh sizes, and extrapolating to zero mesh size. The extrapolated numerical results may then be compared with the analytic results, the c_i. This extrapolation is based on the same idea of "deferred approach to the limit" used[4,5] to obtain the lowest eigenvalue of (2). Some numerical results for the testing of the triplet-odd quadratic spin-orbit term are given.

II. ANALYTIC APPLICATION

In the center-of-mass system for the three nucleons (each of mass M) we introduce the vectors $\vec{r}_{12}$ and $\vec{\rho}$, where

$$\vec{r}_{12} = \vec{r}_1 - \vec{r}_2 , \quad \vec{\rho} = \vec{r}_3 - \tfrac{1}{2}(\vec{r}_1 + \vec{r}_2) .$$

We have then

$$H^s = -\frac{3}{4}\frac{\hbar^2}{M}\nabla_\rho{}^2 - \frac{\hbar^2}{M}\nabla_{r_{12}}{}^2 + V_{12} . \tag{5}$$

In the following, $Y_m^l(\hat{x})$ (where $\hat{x}$ is a unit vector) denotes a spherical harmonic (m is the z component of l), $X^{s_{12}}_{m_{s12}}$ denotes a two-nucleon spin state and $X^{s_3}_{m_{s3}}$ a single-nucleon spin state.

Since we only wish to illustrate how the triplet-odd contribution may be tested, the following discussion is particularized to this case. The relevant expressions for the case where the two-nucleon wave function is a singlet spin state ($s_{12}=0$) are obvious from the expressions for the triplet case.

Two-nucleon triplet spin-state wave functions ($s_{12}=1$) of total angular momentum j_{12} may be defined as follows:

$$W^{j_{12}s_{12}}_{m_{j12}} = \frac{u(r_{12})}{r_{12}} Y^{j_{12}l_{12}^-s_{12}}_{m_{j12}} + \frac{w(r_{12})}{r_{12}} Y^{j_{12}l_{12}^+s_{12}}_{m_{j12}} , \tag{6}$$

$l_{12}^+ = j_{12}+1$, $l_{12}^- = j_{12}-1$. In (6) the Y are defined by

$$Y^{j_{12}l_{12}s_{12}}_{m_{j12}} = \sum_{m_{l12}m_{s12}} \langle l_{12}s_{12}m_{l_{12}}m_{s_{12}} | j_{12}m_{j_{12}}\rangle \times Y^{l_{12}}_{m_{l12}} X^{s_{12}}_{m_{s12}} .$$

The coefficients are the usual Clebsch-Gordan coefficients.[8] The functions u and w are arbitrary.

A three-nucleon state of definite total angular

momentum $\vec{J}$ is obtained by coupling in the spin $\vec{s}_3$ of the third nucleon and then its orbital angular momentum $\vec{l}_3$. We define successively $\vec{K}=\vec{j}_{12}+\vec{s}_3$ and $\vec{J}=\vec{K}+\vec{l}_3$. We define

$$\Phi^{JKl_3}_{m_J}=\frac{F(\rho)}{\rho}\sum_{m_{l3}m_K m_{s3}m_{j12}}\langle Kl_3m_Km_{l_3}|Jm_J\rangle \times\langle j_{12}s_3m_{j_{12}}m_{s_3}|Km_K\rangle \times W^{j_{12}s_{12}}_{m_{j12}}X^{s_3}_{m_{s3}}\,Y^{l_3}_{m_{l3}}(\hat{\rho})\,. \tag{7}$$

The function $F(\rho)$ is arbitrary. To obtain a three-nucleon wave function, (7) must be multiplied by an appropriate isospin function for three nucleons. We use the isospin functions of Blatt,[9] and since we want $T=\frac{1}{2}$ the appropriate function is either v_1 or v_2. The three-nucleon isospin functions v_1 and v_2 are defined in Ref. 9, Eq. (A2); v_1 has nucleons 1 and 2 in the triplet isospin state; v_2, in the singlet isospin state. Finally, then, we define the function ϕ which we shall use in our test:

$$\phi=\Phi^{JKl_3}_{m_J}v_t\,. \tag{8}$$

$F(\rho)$, $u(r_{12})$, and $w(r_{12})$ are arbitrary functions, but for convenience of calculation we shall take

$$F(\rho)=e^{-\gamma\rho},\quad u(r_{12})=e^{-\beta r_{12}},\quad w(r_{12})=e^{-\beta r_{12}}\,.$$

The calculation of $H^s\phi$ is straightforward, using (5):

$$H^s\phi=\frac{3}{4M}\hbar^2\left(\gamma^2-\frac{l_3(l_3+1)}{\rho^2}\right)\phi+\frac{F(\rho)}{\rho}v_t\sum_{m_{l3}m_Km_{s3}m_{j12}}\langle Kl_3m_Km_{l_3}|Jm_J\rangle\langle j_{12}s_3m_{j_{12}}m_{s_3}|Km_K\rangle X^{s_3}_{m_{s3}}Y^{l_3}_{m_{l3}}(\hat{\rho})\times(H_DW^{j_{12}s_{12}}_{m_{j12}})\,,$$

where $H_D=-(\hbar^2/M)\nabla_{r_{12}}{}^2+V_{12}$.

For the case of the Hamada-Johnston potential, the action of H_D on $W^{j_{12}s_{12}}_{m_{j12}}$ may be obtained using Eqs. (5), (6), and (7) in Ref. 10. The result is of the form

$$a(r_{12})Y^{j_{12}l_{12}s_{12}}_{m_{j12}}+d(r_{12})Y^{j_{12}l'_{12}s_{12}}_{m_{j12}}\,.$$

With the above choice of u and w we have

$$a(r_{12})=\left[-\frac{\hbar^2}{M}\beta^2+\frac{\hbar^2}{M}\frac{j_{12}(j_{12}-1)}{r_{12}{}^2}+V_C-\frac{2(j_{12}-1)V_T}{(2j_{12}+1)}+(j_{12}-1)V_{LS}+(j_{12}-1)V_{LL}+\frac{6\sqrt{j_{12}}(j_{12}+1)V_T}{(2j_{12}+1)}\right]\frac{e^{-\beta r_{12}}}{r_{12}}\,,$$

$$d(r_{12})=\left[-\frac{\hbar^2}{M}\beta^2+\frac{\hbar^2}{M}\frac{(j_{12}+1)(j_{12}+2)}{r_{12}^2}+V_C-\frac{2(j_{12}+2)}{(2j_{12}+1)}V_T-(j_{12}+2)V_{LS}-(j_{12}+2)V_{LL}+\frac{6\sqrt{j_{12}}(j_{12}+1)V_T}{(2j_{12}+1)}\right]\frac{e^{-\beta r_{12}}}{r_{12}}\,. \tag{9}$$

The different V's occurring are the different potential term functions (central, tensor, spin-orbit, and quadratic spin-orbit) and should further be differentiated by a label indicating whether they are the triplet-even, triplet-odd, singlet-even, or singlet-odd functions.

We have then

$$H^s\phi=\frac{3}{4M}\hbar^2\left[\gamma^2-\frac{l_3(l_3+1)}{\rho^2}\right]\phi+\frac{e^{-\gamma\rho}}{\rho}v_ta(r_{12})\sum_{m_{l3}m_{s3}m_Km_{j12}}\langle Kl_3m_Km_{l_3}|Jm_J\rangle\langle j_{12}s_3m_{j_{12}}m_{s_3}|Km_K\rangle X^{s_3}_{m_{s3}}Y^{l_3}_{m_{l3}}(\hat{\rho})Y^{j_{12}l_{12}s_{12}}_{m_{j12}}$$
$$+\frac{e^{-\gamma\rho}}{\rho}v_td(r_{12})\sum_{m_{l3}m_Km_{s3}m_{j12}}\langle Kl_3m_Km_{l_3}|Jm_J\rangle\langle j_{12}s_3m_{j_{12}}m_{s_3}|Km_K\rangle X^{s_3}_{m_{s3}}Y^{l_3}_{m_{l3}}(\hat{\rho})Y^{j_{12}l'_{12}s_{12}}_{m_{j12}}\,. \tag{10}$$

The following type of term occurs in both ϕ and $H^s\phi$:

$$v_t\sum_{m_{l3}m_Km_{s3}m_{j12}}\langle Kl_3m_Km_{l_3}|Jm_J\rangle\langle j_{12}s_3m_{j_{12}}m_{s_3}|Km_K\rangle Y^{j_{12}l_{12}s_{12}}_{m_{j12}}X^{s_3}_{m_{s3}}Y^{l_3}_{m_{l3}}(\hat{\rho})\,. \tag{11}$$

That the two conditions (i) and (ii) of Sec. I can be met follows from the paper by Davies,[6] who shows how (11) may be expressed in form (1), given that l_{12} and l_3 satisfy certain conditions, and $J=\frac{1}{2}$. (Davies also considers the $J=\frac{3}{2}$ case, for which an expansion of form (1) is also possible, but with more terms.) The first step in this is to recouple the angular momenta to the more symmetrical order

$$\vec{J}=(\vec{l}_{12}+\vec{l}_3)+(\vec{s}_{12}+\vec{s}_3)\,.$$

This may be done by the standard methods using

6-j symbols,[8] and (11) may be expressed as a linear combination of states of definite L and S, $\psi(l_{12}l_3L;s_{12}s_3S;J)$. Davies in Eq. (20) gives the formula only for the cases l_{12} equal to 0 and 2. The general expression for the expansion of (11) is

$$v_t \sum_{L,S} (-1)^{l_{12}+s_{12}+s_3+l_3-L-S} \times [(2K+1)(2S+1)(2L+1)(2j_{12}+1)]^{1/2} \times \begin{Bmatrix} S & l_{12} & K \\ l_3 & \frac{1}{2} & L \end{Bmatrix} \begin{Bmatrix} l_{12} & s_{12} & j_{12} \\ \frac{1}{2} & K & S \end{Bmatrix} \psi(l_{12}l_3L;s_{12}s_3S;J). \tag{12}$$

In Eq. (25) Davies shows how $v_t\psi(l_{12}l_3L;s_{12}s_3S;J)$ may be expressed as a linear combination of the $\mathcal{Y}_i$ of Eq. (1).

To summarize, we have shown that, for the form of ϕ chosen, $\hat{H}\phi$ can be evaluated using the matrix H. $H^s\phi$ is easily evaluated independently, and the comparison of $\hat{H}\phi$ and $H^s\phi$ follows directly by comparison of the coefficients in the respective expansions in the $\mathcal{Y}_i$.

We shall illustrate the testing of the triplet-odd quadratic spin-orbit contribution to H.

A. Derivation of appropriate ϕ

By choosing the two-particle state to be triplet-odd the different V's occurring in $a(r_{12})$ and $d(r_{12})$ will be the triplet-odd parts of the respective potentials. Choosing the two-particle state $^3P_0$, we have

$$j_{12}=0, \quad l_{12}=1, \quad s_{12}=1,$$

hence

$$K=\tfrac{1}{2}.$$

The requirement of even parity for the three-nucleon function requires that l_3 equal 1. The relevant isospin function is v_2 and the four functions occurring in (12) are $\psi(1\,1\,0;1\,\frac{1}{2}\,\frac{1}{2};\frac{1}{2})$, $\psi(1\,1\,1;1\,\frac{1}{2}\,\frac{1}{2};\frac{1}{2})$, $\psi(1\,1\,1;1\,\frac{1}{2}\,\frac{3}{2};\frac{1}{2})$, and $\psi(1\,1\,2;1\,\frac{1}{2}\,\frac{3}{2};\frac{1}{2})$. Using Davies [Eq. (25)] we obtain for the expansion of ϕ

$$\phi=\frac{e^{-\gamma\rho}}{\rho}\frac{w(r_{12})}{r_{12}}\left[\frac{1}{2\sqrt{3}}\cos\eta(\mathcal{Y}_2-\mathcal{Y}_{3,1}) - \frac{1}{2\sqrt{3}}\sin\eta(\mathcal{Y}_4+\mathcal{Y}_{6,2}+\mathcal{Y}_{7,2}) - \frac{1}{2\sqrt{3}}\cos\eta\mathcal{Y}_{8,1} - \tfrac{1}{2}\cos(\eta-2\theta)\mathcal{Y}_{9,2} + \tfrac{1}{2}\sin(\eta-2\theta)\mathcal{Y}_{10,2}\right]. \tag{13}$$

The labeling scheme for the $\mathcal{Y}$'s is that of Derrick,[2] and $\cos\eta$, etc., are functions of the interparticle distances, also given by Derrick. The following corrections should be made in Davies's Appendix I, where he tabulates the expansion coefficients occurring in his Eq. (25): $C_{0s}^{202}=(3\sqrt{5}/4\sqrt{7})(\cos2\eta-\frac{1}{3})$, $D_{1m1}^{1\,\frac{1}{2}\,\frac{1}{2}}=1/\sqrt{2}$ and C_{2s}^{222}, C_{2a}^{222} have the wrong sign. Davies's spin functions $X_{m_s}^{s_{12}s_3S}$ are related to the spin functions of Derrick and Blatt[1] (Appendix 2) by

$$X_{\frac{1}{2}}^{1\,\frac{1}{2}\,\frac{1}{2}}=-q_1, \quad X_{\frac{1}{2}}^{0\,\frac{1}{2}\,\frac{1}{2}}=-q_2, \quad X_{\frac{1}{2}}^{1\,\frac{1}{2}\,\frac{3}{2}}=q_3.$$

In the definition of $V_{m_sk'}^{s}(P_s,T)$ given by Kalotas and Delves[11] in Eq. (2), the spin function occurs before the isospin function. This differs from the convention of Derrick and Blatt and means that $V_{\frac{1}{2}\,1}^{\frac{1}{2}}(a,\frac{1}{2},\frac{1}{2})$ is $-V_{\frac{1}{2}}^{\frac{1}{2}}(a,\frac{1}{2},\frac{1}{2})$. Davies uses $V_{\frac{1}{2}}(a,\frac{1}{2},\frac{1}{2})$, not $V_{\frac{1}{2}\,1}^{\frac{1}{2}}(a,\frac{1}{2},\frac{1}{2})$, in Eq. (25).

B. Calculation of $H^s\phi$

With the results in Sec. II A we can check all the triplet-odd contributions to H. The different terms (kinetic energy, central potential, etc.) can be tested separately by setting all the others to zero. Consider the quadratic spin-orbit potential term and let V denote the quadratic spin-orbit triplet-odd potential function. The coefficient of $\mathcal{Y}_{10,2}$ in $H^s\phi$ (i.e., c_{16}) is $-\sin(\eta-2\theta)Ve^{-\beta r_{12}}e^{-\gamma\rho}/r_{12}\rho$, since l_{12} is $j_{12}+1$, $a(r_{12})$ is zero, and $d(r_{12})$ is $-2Ve^{-\beta r_{12}}/r_{12}$.

C. Calculation of $\hat{H}\phi$ using H

Using Derrick's matrix H calculated with the unmodified D states,[2,3] we can obtain $\sum_j H_{16j}g_j$ (i.e., b_{16}), the coefficient of $\mathcal{Y}_{10,2}$ in $\hat{H}\phi$, when the other terms besides the quadratic spin-orbit term have been set to zero. The result is

$$\left\{-\frac{2}{\sqrt{3}}\frac{\sin(2\theta-\eta)}{\sin\eta}B\left(\frac{1}{2\sqrt{3}}\cos\eta\right)-\tfrac{3}{4}\sin(\eta-2\theta)+(-c)\left(-\frac{1}{2\sqrt{3}}\cos\eta\right)+E[-\tfrac{1}{2}\cos(\eta-2\theta)]+2e[\tfrac{1}{2}\sin(\eta-2\theta)] + \tfrac{4}{3}dC^+\left(-\frac{1}{2\sqrt{3}}\cos\eta\right)+\tfrac{4}{3}dc[-\tfrac{1}{2}\cos(\eta-2\theta)]+\tfrac{4}{3}d^2\tfrac{1}{2}\sin(\eta-2\theta)\right\} V\frac{e^{-\beta r_{12}}}{r_{12}}\frac{e^{-\gamma\rho}}{\rho}=-\sin(\eta-2\theta)V\frac{e^{-\beta r_{12}}}{r_{12}}\frac{e^{-\gamma\rho}}{\rho}.$$

The quantities θ, η, e, c, and d are functions of r_{12}, r_{23}, and r_{13}, and B, C^+, and E involve first-order derivatives in these variables. For the definitions see Derrick's papers.

Agreement between the results of the two calculations (Secs. II B and II C) checks the triplet-odd

contribution of the quadratic spin-orbit term potential to the matrix elements in the 16th row of H. Proceeding in the same way, we could check all the contributions of all the terms of the potential to all the matrix elements. The functions ϕ used in the testing of the other spin-parity states and their expansions are: (i) *Triplet-even.* These are given expanded in the $\psi(l_{12}l_3L; s_{12}s_3S, J)$ by Davies in Appendix 4; (ii) *Singlet-even.* We used the $^1D_2$ state and so the functions occurring are $\psi(2\,2\,0; 0\,\frac{1}{2}\,\frac{1}{2}; \frac{1}{2})$ and $\psi(2\,1\,1; 0\,\frac{1}{2}\,\frac{1}{2}; \frac{1}{2})$; we have

$$\phi = \frac{e^{-\gamma\rho}}{\rho}\frac{u(r_{12})}{r_{12}}\left[-\frac{3}{4\sqrt{2}}(\cos 2\eta + \tfrac{1}{3})(\mathcal{Y}_1 + \mathcal{Y}_{3,2}) + \tfrac{1}{4}\sqrt{\tfrac{5}{3}}\sin 2\eta(\mathcal{Y}_5 + \mathcal{Y}_{6,1})\right];$$

(iii) *Singlet-odd.* We used the $^1P_1$ state and so the functions occurring are $\psi(1\,1\,0; 0\,\frac{1}{2}\,\frac{1}{2}; \frac{1}{2})$ and $\psi(1\,1\,1; 0\,\frac{1}{2}\,\frac{1}{2}; \frac{1}{2})$. We have

$$\phi = \frac{e^{-\gamma\rho}}{\rho}\frac{u(r_{12})}{r_{12}}\left[\tfrac{1}{2}\cos\eta(\mathcal{Y}_2 + \mathcal{Y}_{3,1}) - \tfrac{1}{2}\sin\eta(\mathcal{Y}_4 + \mathcal{Y}_{6,2})\right].$$

III. NUMERICAL APPLICATION

In our numerical method for solving (2), the matrix H is replaced at each point by a finite-difference representation in which the operators are replaced by finite-difference formulas. We can test both our finite-difference representation of H and our programming of it by performing a numerical version of the analytic test described in the previous section. The 16 functions g_i in the expansion of ϕ may be represented by a three-dimensional array of numbers and, on a particular mesh size, an approximation to Hg at a particular point in space may be obtained by acting with the representation of H on the numerical version of g.

Setting V_{23} and V_{13} to zero in the finite-difference version of H, we can calculate, at a particular point on a particular mesh size, 16 numbers which are approximations to $b_1 - b_{16}$. By extrapolating to zero mesh size the numerical results calculated for a particular point (corresponding to fixed values of r_{12}, r_{23}, and r_{13}), we can get an estimate for the analytic results at that point (which are given by $c_1 - c_{16}$). The two results typically agreed to about six figures for the meshes we used and this was taken as sufficient accuracy for checking. In setting up our numerical Hamiltonian we actually used the matrix elements calculated with the modified D states[13] so that the test also checks the work involved in obtaining these.

Particular terms of the Hamada-Johnston potential are tested by setting the other terms to zero in the program and the different contributions to each term (triplet-odd, etc.) by corresponding choice of a two-nucleon state, as described in Sec. II. In this way we were able to carry out a complete check of the programming of the Hamada-Johnston potential in the program that was used to compute the eigenvalues. The test may be adaptable by other workers in the three-nucleon field and used to check their own representations of the triton Hamiltonian.

Table I illustrates the testing of the triplet-odd part of the quadratic spin-orbit term of the potential. The extrapolation table gives the extrapolated value for b_{16}. The first column gives the estimates for b_{16} for various mesh sizes h. The remaining columns contain extrapolations to $h = 0$. The leading term in the error of the estimates of the analytic result in the nth column is proportional to h^n, and the most accurate estimates of the limit occur on the lowest line of the table,

TABLE I. Example of the extrapolation of a series of numerical estimates of b_{16} to zero mesh size, $h = 0$.

h	Estimate					
$\frac{1}{16}$	−2.153 701 0					
		−2.335 632 6				
$\frac{1}{32}$	−2.244 666 8		−2.343 474 5			
		−2.340 860 5		−2.344 820 6		
$\frac{1}{48}$	−2.276 731 4		−2.344 484 1		−2.344 925 1	
		−2.342 672 3		−2.344 904 2		−2.344 928 8
$\frac{1}{64}$	−2.293 216 6		−2.344 736 2		−2.344 928 2	
		−2.343 497 9		−2.344 920 2		
$\frac{1}{80}$	−2.303 272 9		−2.344 828 2			
		−2.343 941 3				
$\frac{1}{96}$	−2.310 050 9					

since these pertain to the finest mesh sizes. The analytic result for comparison, obtained from $H^s\phi$, is $-2.344\,928\,9$ [the value of $-\sin(\eta - 2\theta)\, V(e^{-\beta r_{12}}/r_{12})(e^{-\gamma\rho}/\rho)$, i.e., c_{16}]. All results were printed out to eight figures.

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[1]G. Derrick and J. M. Blatt, Nucl. Phys. 8, 310 (1958).
[2]G. Derrick, Nucl. Phys. 16, 405 (1960).
[3]G. Derrick, Nucl. Phys. 34, 543 (1962).
[4]I. M. Bassett and B. R. E. Lederer, Phys. Lett. 32B, 550 (1970).
[5]I. M. Bassett, B. R. E. Lederer, and G. C. Vorlicek, Phys. Lett. 51B, 329 (1974).
[6]B. Davies, Nucl. Phys. 88, 361 (1966).
[7]B. Davies, Nucl. Phys. 79, 427 (1966).
[8]A. Edmonds, *Angular Momentum in Quantum Mechanics* (Princeton U.P., Princeton, 1957).
[9]J. M. Blatt, Phys. Rev. 89, 86 (1953).
[10]T. Hamada and I. Johnston, Nucl. Phys. 34, 382 (1962).
[11]T. Kalotas and L. M. Delves, Nucl. Phys. 60, 363 (1964).
[12]L. Cohen and J. B. Willis, Nucl. Phys. 32, 114 (1962).
[13]G. Derrick, Nucl. Phys. 18, 303 (1960).