Matrix solution of the Bethe-Faddeev equations*

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The Bethe-Faddeev equations are set up in matrix form and solved for the ^{3}H nucleus. The two-body g matrix is derived from a revised version of the Brueckner-Bethe-Goldstone formalism. Application to the Reid soft core potential indicates that this interaction yields an eigenvalue very close to the experimental binding energy of ^{3}H.

[NUCLEAR STRUCTURE Three-body correlations, Brueckner-Bethe-Goldstone method, binding energy, ^{3}H, Reid and Hamada-Johnston potentials.]

I. INTRODUCTION

Calculations using the Brueckner-Bethe-Goldstone formalism have yielded very encouraging results on nuclear matter and finite nuclei. The literature on this subject has become extensive, and excellent reviews of the early work are available.[1-3] The goal of such procedures is to perfect the accuracy of the calculations until definitive conclusions can be reached concerning the validity of specific nucleon-nucleon interaction operators.

The purpose of this paper is to investigate a method for calculating the ground state binding energy of the three nucleon system which combines the g matrix formalism with the Bethe-Faddeev[3,4] equations, and which can be extended to heavier nuclei. In order to attempt precise results for ^{3}H, some elementary alterations of the established procedures are made, which appear to be appropriate for such a light nucleus.

II. FORMALISM

The nonrelativistic Hamiltonian for the three-body system with general two-body forces V_{ij} is given in the familiar form,

$$H = \sum_i T_i + \sum_{i<j} V_{ij} - T_{\text{c.m.}} \ . \tag{2.1}$$

Let us start by rewriting this Hamiltonian as

$$H = H_0 + W - H_0^{\text{c.m.}} \ , \tag{2.2}$$

where we use the following definitions:

$$H_0 = (\hbar^2/2m) \sum_i p_i{}^2 + \sum_i U_i \ , \tag{2.2a}$$

$$W = \sum_{i<j} W_{ij} = \sum_{i<j} (V_{ij} - U_{ij}) \ , \tag{2.2b}$$

$$U_i = \tfrac{1}{2}\omega^2 m r_i{}^2 \ , \tag{2.2c}$$

and

$$\sum U_{ij} = \tfrac{1}{2}\omega^2 m \sum_i \left(\vec{\mathrm{r}}_i - A^{-1} \sum_j \vec{\mathrm{r}}_j \right)^2$$

$$= (\omega^2 m/2A) \sum_{i<j} (\vec{\mathrm{r}}_i - \vec{\mathrm{r}}_j)^2 \ . \tag{2.2d}$$

The form of Hamiltonian has been previously employed in perturbation calculations[5,6] on light nuclei. It does not represent any distortion of Eq. (2.1), as one has simply rearranged terms.

The two-body g matrix can now be defined by

$$g_{ij} \equiv W_{ij} + W_{ij} \frac{Q}{e} g_{ij} \ , \tag{2.3}$$

where

$$\frac{Q}{e} \equiv \sum_n{}' \frac{|n\rangle\langle n|}{E - (H_0 - H_0^{\text{c.m.}})} \ . \tag{2.3a}$$

The prescription for Q/e used here differs from that given by the linked cluster expansion. The value of E in Eq. (2.3a) is given as the energy eigenvalue which we seek. Consequently one is generating the Brillouin-Wigner perturbation series, which in the case for ^{3}H does not differ significantly from the Block-Horowitz[7] expansion for open shell nuclei. We must then continue to generate the remaining terms in the Brillouin-Wigner perturbation series, a point which must be kept in mind for the remainder of this paper.

First we must compute the matrix elements of g_{ij}. It is not practical to do this entirely by the usual procedures. The difficulty is that W_{ij} retains U_{ij} as well as V_{ij}, and U_{ij} is a very long range potential. Hence if one attempts to compute a correlated wave function corresponding to W_{ij} directly from the Bethe-Goldstone equation, the wound function does not heal properly.

This difficulty is nontrivial and actually essential (in one form or another) to any attempt at precision when one is perturbing harmonic oscillator orbitals into nuclear wave functions. Oscillator wave functions have a Gaussian assymptotic form, while the nuclear wave functions doubtlessly are closer to an exponential dependence at large nucleon-nucleon separations. A correction for this must appear somewhere in the formalism.

As a first step in deducing g_{ij}, we solve the Bethe-Goldstone equation without U_{ij} in reference spectrum[8] approximation (Q set equal to unity):

$$\psi = \varphi + e^{-1} V_{ij}\psi \tag{2.4}$$

and then calculate

$$\langle\varphi| g_{ij}^R |\varphi\rangle = \langle\varphi| V_{ij} |\psi\rangle \ . \tag{2.5}$$

Next one constructs the set of matrix equations,

$$g'_{ij} = g_{ij}^R + g_{ij}^R \left(\frac{Q}{e'} - \frac{1}{e}\right) g'_{ij}$$

$$= \left[1 - g_{ij}^R \left(\frac{Q}{e'} - \frac{1}{e}\right)\right]^{-1} g_{ij}^R \ , \tag{2.6}$$

where

$$e' = E - H_0 + H_0^{\text{c.m.}} + QU_{ij}Q \ . \tag{2.6a}$$

Equation (2.6) corrects the g matrix elements for the neglect of the Pauli principle in Eq. (2.4). Furthermore by inserting the term $QU_{ij}Q$ into e', one inserts an infinite sequence of $-U_{ij}$ terms between any two V_{ij} terms:

$$\frac{Q}{e'} = \frac{Q}{e + QU_{ij}Q}$$

$$= \frac{Q}{e} - \frac{Q}{e}U_{ij}\frac{Q}{e} + \frac{Q}{e}U_{ij}\frac{Q}{e}U_{ij}\frac{Q}{e} - \cdots \ . \tag{2.7}$$

The only remaining correction is to include all diagrams which begin or end with a $-U_{ij}$ term; so the final expression for g_{ij} becomes

$$g_{ij} = \left(1 + U_{ij}\frac{Q}{e}\right)^{-1} g'_{ij} \left(1 + \frac{Q}{e}U_{ij}\right)^{-1}$$

$$- U_{ij}\left(1 + \frac{Q}{e}U_{ij}\right)^{-1} \ . \tag{2.8}$$

Equations (2.6)–(2.8) are solved simply by setting up matrices for g_{ij}, U_{ij}, Q, e, and e' in an oscillator basis. All indicated operations are then performed by standard procedures of matrix multiplication and inversion.[9] All matrices are of infinite order, and consequently must be truncated at some finite order. Truncations of this type are the only approximations made in this study. The convergence of such a procedure has previously been investigated by Sauer,[10] who demonstrates that even though matrices like that for $QU_{ij}Q$ (in his paper it is actually QTQ) diverge, only a relatively low order in the matrix is needed to obtain an accurate value for the first few terms in the inverse. In this investigation we have verified his conclusions.

This method may have application beyond the example given here, in that it shows how an interaction with both short and long ranged components may be treated in the g matrix formalism. There is a catch, however, and rather a big one. By introducing long range components into W_{ij}, one may also have induced sizable three-body correlations. Therefore a construction of the g matrix such as we have above should never be attempted unless one also intends to solve the Bethe-Faddeev equations:

$$T_3 = g_{12} + g_{12}\frac{Q}{e}(T_1 + T_2) \tag{2.9}$$

(and cylic permutations).

Our method of solution for Eq. (2.9) is very similar to the method of solution for Eqs. (2.6) and (2.8) described above, and involves exactly the same approximation. One already has g_{12}, Q, and e in matrix form, ready to apply the needed operations.

The basis, in all of our matrix solutions, is set up very easily. We use the Jacobi coordinates:

$$\vec{\rho} = \frac{1}{\sqrt{2}}(\vec{r}_1 - \vec{r}_2) \ ,$$

$$\vec{\zeta} = \frac{1}{\sqrt{6}}(\vec{r}_1 + \vec{r}_2 - 2\vec{r}_3) \ ,$$

and

$$\vec{R} = \frac{1}{\sqrt{3}}(\vec{r}_1 + \vec{r}_2 + \vec{r}_3) \ . \tag{2.10}$$

The orbital part of the basis then has the form

$$\Phi_{nlmn'l'm'} = \phi_{nlm}(\vec{\rho})\phi_{n'l'm'}(\vec{\zeta})\phi_{000}(\vec{R}) \ . \tag{2.11}$$

Quite naturally one wants to keep the center of mass motion in the 0s state, where it makes very little trouble. One can then replace $H_0^{\text{c.m.}}$ everywhere above by just $\frac{3}{2}\hbar\omega$. The ϕ_{nl} are just the oscillator functions. The basis is completed by first vector coupling the Φ together to obtain a basis where the total number of oscillator quanta ($N = 2n + 2n' + l + l'$), the total orbital angular momentum (L), and the orbital symmetry ($[\lambda]$) are good quantum numbers. Then one must vector couple the result to spin-isospin vectors to obtain a final basis which is antisymmetric under the interchange of any two nucleons, and consistant with the absolute quantum numbers of ^{3}H. The process has been previously described in detail by Aguilera Navarro, Moshinsky, and Yeh.[11]

An additional simplification is now possible.

Since we consistently deal with an antisymmetric basis we have

$$g_{12} = g_{13} = g_{23} = g \tag{2.12}$$

and

$$T_1 = T_2 = T_3 = t \ . \tag{2.13}$$

Equations (2.12) and (2.13) hold so long as we clearly imply that g and t stand for the matrix elements of the operator, and are therefore just sets of numbers. It is also important to note that the three-body basis defining Q is used not only in the Bethe-Faddeev equations [Eq. 2.9)] but also in the Pauli correction to the two-body g matrix [Eqs. (2.6) and (2.8)]. Thus we consistently employ a "Brillouin-Wigner" Pauli operator, as opposed to the Brueckner definition of Q.

A pedantic point should be made here. When one employs the three-body Pauli operator Q, the states $P = 1 - Q$ are not all antisymmetric. Certainly one must prohibit scattering into such states, and this must be accounted for in Eq. (2.6) when one sets up the matrix for $1/e$. Consequently the Pauli corrected g matrix in this paper includes an "antisymmetrization correction" which is generally included in higher orders of the conventional Brueckner-Bethe-Goldstone calculations.

Once this correction is included, the three coupled Bethe-Faddeev equations reduce to just one equation:

$$t = g + 2g\frac{Q}{e}t$$

$$= \left(1 - 2g\frac{Q}{e}\right)^{-1} t \ . \tag{2.14}$$

The energy eigenvalue for ^{3}H is then given by solving the implicit equation:

$$E = \langle \Phi_{0000} | H_0 + 3t(E) | \Phi_{0000} \rangle - \tfrac{3}{2}\hbar\omega \ . \tag{2.15}$$

III. RESULTS

The first question one must answer in performing the calculations is that of truncating the basis. We attempted several experiments. For example one can include only the $[\lambda] = [3]$ S states up to a rather high value for the number of oscillator quanta (N), or suppress all the P states. We found such approximations often to be misleading. It is very hard to put a value on the contribution of a particular state because of the importance of cross terms in the matrix inversion process. Thus, for example, the contribution made by adding on a particular state to the basis depends very strongly on which states have gone before it. The final procedure we decided on (and presented here) is very straightforward. One simply takes all states corresponding to a particular number of oscillator quanta, and proceeds to include higher N until one has convergence.

Results for the Hamada-Johnston (HJ)[12] and Reid[13] soft core (RSC) interactions are shown in Tables I and II. Values listed for $N = 0$, of course, include only two-body correlations. All numbers are subject to a maximum computational error of 30 keV, which could be removed by performing the calculation in double precision.

Does the procedure converge as N is increased? The binding energy changes by nearly 1 MeV when one goes from $N = 4$ to $N = 6$, which does not (at first glance) instill confidence. There are several points to be considered, however. First, let us note that it is not possible to rigorously establish convergence of a series without examining its analytic properties. Even if the basis states in $N = 6$ had made a very small contribution to the energy, that in itself would be a poor reason to conclude that the calculation has converged.

The contribution of the $N = 6$ basis states is far less impressive when one considers the size of the function space involved. There is one state with $N = 0$ (not in Q), 4 states with $N = 2$, 10 with $N = 4$, and 19 with $N = 6$. Thus when one goes from $N = 4$ to $N = 6$ one goes from a function space with 14 states in Q to a function space with 33 states in Q. Since the size of the basis has more than doubled, an increase in binding is not too surprising. Furthermore, the comparatively small change in energy at $N = 2$ is characteristic of calculations in an oscillator basis, as noted by other authors.[23]

In the course of this work we have generated g matrix elements up to $N = 22$. Examination of these matrix elements as a function of N indicates that the trend established in the numbers presented here will continue for higher N, and the remainder is small.

As a final check on the revised g-matrix formalism presented in Sec. II one may calculate the binding energy of ^{2}H. Although this is a most elementary application, it can be valuable as the result can be compared both with an exact answer and a variational procedure that has also been applied to ^{3}H.

TABLE I. Binding energies (in MeV) for the Reid soft core potential.

	$\hbar\omega$ (MeV)		
N	8	10	12
0	4.16	4.57	4.59
2	5.32	5.51	5.45
4	7.10	7.36	7.37
6	8.21	8.37	8.35

TABLE II. Binding energies (in MeV) for the Hamada-Johnston potential.

	$\hbar\omega$ (MeV)		
N	8	10	12
0	3.96	4.23	4.09
2	5.01	5.03	4.81
4	6.62	6.73	6.58
6	7.56	7.63	7.50

One minor problem arises when applying the formalism to ^{2}H. The appropriate energy denominator to be used in Eq. (2.6) is clearly

$$e' = E - QT_{\rm rel}\,Q$$

after correcting for the Pauli effect and the $-U_{ij}$ insertions. Now one could start the procedure either by using a plane wave propagator in Eq. (2.4):

$$e_1 = E - T_{\rm rel}$$

or with the oscillator propagator:

$$e_2 = E - H_0 + H_0^{\rm c.m.} \ .$$

Both procedures are correct in principle, since one always will use Eq. (2.6) to restore the right energy denominator. If one starts with e_1 one finds excellent convergence toward the exact result, however, and if one starts with e_2 convergence is poor. This point was previously reported in some detail by Sauer,[10] and we will not dwell on it here. The same option is open in the ^{3}H calculation, and can be used as an additional check on convergence. In the triton we found that e' differs only very slightly from either the plane wave or oscillator propagator, and the choice is left to mathematical convenience.

Using e_1 in Eq. (2.4) the g matrix elements generated by Eqs. (2.6) and (2.8) yield accuracy to nearly two significant figures for $N=2$ ($E=-2.14$ MeV), and three good figures for $N=10$ ($E=-2.22$ MeV). We have verified that the RSC potential yields an exact eigenvalue of -2.226 MeV, by direct interaction of the Rarita-Schwinger coupled differential equations.

This convergence rate may be compared with the work of Jackson, Lande, and Sauer,[22] who have performed a variational calculation on the deuteron by expanding the trial wave functions in an oscillator basis. They find that $N=20$ is needed to obtain $E=-1.5$ MeV, and $N=48$ is required to get $E=-2.1$ MeV. Thus the g-matrix approach is seen to exhibit a great advantage over a variational calculation in the same oscillator basis.

IV. COMPARISON WITH OTHER CALCULATIONS AND WITH EXPERIMENT

The experimental binding energy of ^{3}H is 8.48 MeV. The results of Sec. III imply that the RSC[13] interaction yields a very close fit to experiment (probably to within about 200 keV), while the HJ[12] potential yields an eigenvalue which is only about 600 to 900 keV short. Unfortunately one can come to no definite conclusion as to which two-body potential is best due to the uncertain magnitude of relativistic effects and three-body forces.

Several other calculations[14-22] have been performed on ^{3}H using the RSC and HJ potentials, generally yielding binding energies between 6 and 8 MeV. The best variational calculation for the HJ potential was performed by Delves and Hennell,[18] who obtained an upper bound of -6.55 ± 0.25 MeV with a corresponding lower bound of -41.2 ± 20 MeV. Our estimated eigenvalue is well within these limits. In order to obtain the lower bound, Delves and Hennell calculated $\langle H^2\rangle$ with their trial wave function, and the value of this parameter is therefore available in their paper. This value for $\langle H^2\rangle$ can be used to make a crude estimate of the effect on the energy eigenvalue that might be attained by introducing additional variational flexibility into the trial wave function. Define:

$$\varphi' = \varphi + \lambda H\varphi \ , \tag{4.1}$$

where λ is a variational parameter. To compute a new approximation to the energy, one just needs $\langle\varphi|H|\varphi\rangle$, $\langle\varphi|H^2|\varphi\rangle$, and $\langle\varphi|H^3|\varphi\rangle$. The expectation value of H^3 is not available, but can be approximated by

$$\langle\varphi|H^3|\varphi\rangle \approx \langle\varphi|H|\varphi\rangle\langle\varphi|H^2|\varphi\rangle \ . \tag{4.2}$$

Equation (4.2) becomes exact in the limit when φ is an eigenfunction of H, and thereby one estimates a lower limit on the magnitude of the new variation with this approximation. We can then write

$$\delta E \equiv \frac{\langle\varphi'|H|\varphi'\rangle}{\langle\varphi'|\varphi'\rangle} - \langle\varphi|H|\varphi\rangle \tag{4.3}$$

which after variation of λ and use of Eq. (4.2) becomes approximately,

$$\delta E \approx \frac{\langle\varphi|H^2|\varphi\rangle - \langle\varphi|H|\varphi\rangle^2}{2\langle\varphi|H|\varphi\rangle} < -0.7 \text{ MeV} \ . \tag{4.4}$$

The inequality in Eq. (4.4) is set by the fact that we have used the smallest value of $\langle H^2\rangle$ within the error bars of Delves and Hennell. As a consequence it would certainly appear that there is no disagreement between our eigenvalue estimate

for the Hamada-Johnston potential and the variational calculations.

Hennell and Delves[17] compute a variational upper bound for the RSC potential of -7.75 ± 0.5 MeV. A value for $\langle H^2 \rangle$ has not yet been reported, probably because of the large error estimated in $\langle H \rangle$. We note, however, that for both the RSC and HJ potentials we estimate an eigenvalue on the order of 1 MeV lower than the best bounds computed. Thus, at least, one has consistency.

All calculations for the RSC potential involving solution of the Faddeev equations (not to be confused with the Bethe-Faddeev equations examined in this paper) seem to yield results near -7 MeV.[14-16,21,22] Laverne and Gignoux[14] construct a solution by direct integration of the Faddeev equations in configuration space, retaining only the $^1S_0$, $^3S_1$, and $^3D_1$ partial waves in the interaction. They obtain an eigenvalue of -7.0 MeV, which is then shifted to -7.18 MeV when the $^3P_{0,1,2}$ $^1D_2$, and $^3D_2$ partial waves in the interaction are included by perturbation theory. This latter value is just out of the error bars (-7.75 ± 0.5 MeV) defined by the variational investigation.[17]

Laverne and Gignoux[14] point out two possible sources of error in their calculation. The first is the size of the discretization grid, which is also the source of the large error bars in the variational estimate. The second point is the truncation of the Faddeev amplitudes included in the numerical integration procedure. The latter seems most serious to the present authors.

When one expresses the nuclear interaction ($\sum V_{ij}$) in terms of the Jacobi coordinates defined in Eq. (2.10), one finds partial waves corresponding to very high values of the angular momentum from terms like

$$(\vec{\rho} \cdot \vec{\xi})^k \ .$$

Thus when one expands the wave function for H^3 into a series of functions like those in Eq. (2.11), one must find corresponding components with very large values of l and l'. Analysis of the Hennell-Delves trial wave function into Jacobi coordinates reveals such terms, particularly from that part of the wave function that exhibits short range correlations. Consequently the Faddeev solutions must be regarded as a very powerful method of calculation, however when one truncates the Faddeev amplitudes one is clearly dealing with a wave function of limited variational flexibility.

V. CONCLUSIONS

The only approximation made in the present method is the truncation of the basis defining the Brillouin-Wigner Pauli operator Q. The basis is needed to construct the matrices required for the inversion and multiplication operations implied by Eqs. (2.6), (2.8), and (2.14). All of the operators to be inverted produce "band matrices." Band matrices diverge along the main diagonal, but converge rapidly as one considers matrix elements away from the main diagonal. Enlarging the dimension of such matrices has a small effect on the elements of the inverted matrix for small quantum numbers.

Sauer[10] has carefully tested this band matrix theorem for operators of the same general form as those present here. The approximation is consistently very accurate, even when one inverts matrices of relatively small dimension. In the present calculation only one matrix element must be produced accurately [the one in the first row and the first column displayed in Eq. (2.15)]. It must be noted that the present calculation puts considerably more strain on this theorem than those cases tested by Sauer, in that one performs about 3 times as many operations of matrix inversion and multiplication.

The calculation reported here is not variational. Therefore, it could in principle produce too much binding energy, although this is certainly not the trend which appears to be established in all of our calculations. More work is obviously needed before one can assert that precision to two significant figures in the eigenvalue is attained. Variational calculations with improved accuracy and additional variational flexibility could prove most useful, as well as extension of the current work to larger N and further investigation of the Faddeev equations.

The authors also intend to use the general formalism for heavier nuclei, the purpose for which it was originally devised. It may be worth noting that the computer programs for this calculation require only 18 min of processor time on the computational facility available to us, to produce one column in Table I.

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