Comparison between an extended g-matrix formalism and variational calculations in an oscillator basis

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Results obtained with the g-matrix are compared in detail with variational calculations, by restricting both procedures to an oscillator basis consisting of the same maximum number of oscillator quanta. Three-body correlations are included in the g-matrix calculation by extending the basis of the hole states to include additional oscillator functions. The resulting formalism is similar to the Bethe-Faddeev equations, but the correlated wave function is presented in a way to make comparison with variational wave functions obvious. This comparison suggests a choice of potential in the particle states that yield a very small three-body correlation energy in ^{3}H. Applications include the Sussex interaction, and a singular short-range repulsion.

[NUCLEAR STRUCTURE g-matrix and variational calculations, ^{3}H, Sussex interaction, δ-function potential.]

I. INTRODUCTION

The calculation of the properties of complex nuclei with realistic nucleon-nucleon interactions is a fundamental problem of nuclear theory.[1,2] A difficulty in most methods of calculation lies in determining the accuracy of the final results. Of course one generally compares the theoretical values with their experimental counterparts, but then one is left with the dilemma of determining whether any discrepancies are due to the existence of many-body forces, relativistic effects, failure of the two-body potential, or inadequacy in the calculational procedure. Clearly one must have some sort of reasonable estimate of the accuracy of the calculation itself before one can begin to speculate on other sources of discrepancy.

The work reported here represents an attempt to test criteria for the accuracy of the Brueckner-Bethe-Goldstone[2,3] g-matrix method in very light nuclei. This paper will deal only with the simplest of complex nuclei ^{3}H.

The most reliable way to check the accuracy of a calculation is to have an exact answer available for comparison. Analytically soluble potential models of the three-body problem are restricted to such elementary forces, however, that they yield little insight into realistic problems.

The procedure to be used in this paper is to employ realistic forces, but truncate all calculations in a vector space which includes only a certain maximum number of oscillator quanta. A variational calculation in this space will then be referred to as if it were an "exact" result; with which one can compare g-matrix and perturbation calculations subject to the same truncation.

When this comparison is unsatisfactory, three-body correlations must be included in the g-matrix calculation for improvement. A formalism to accomplish this (which is similar to that of Bethe and Faddeev[4-8]) is presented in Sec. II.

II. FORMAL COMPARISON BETWEEN THE VARIATIONAL METHOD AND THE g MATRIX

The Schrödinger equation for the intrinsic nuclear system

$$(H_0+V)\Psi=E\Psi \tag{2.1}$$

can be divided into a set of single-particle operators

$$H_0=\sum_{i=1}^{A} h_i \tag{2.1a}$$

and a two-particle interaction

$$V=\sum_{i<j} v_{ij}\,. \tag{2.1b}$$

In this section we shall take h_i to be the simple harmonic oscillator Hamiltonian. Little use will be made of this assumption, however, since we will later wish to consider the possibility of a better single-particle potential.

The wave function is now taken in the form

$$\Psi=\Phi+\sum_{i<j}\chi_{ij}\,. \tag{2.2}$$

Φ is an appropriately antisymmetric function constructed from oscillator orbitals, which is most conveniently written in bra and ket notation

$$|\Phi\rangle=\sum_{n=0}^{N_0}|n\rangle\langle n|\Psi\rangle\,. \tag{2.3}$$

Each state $|n\rangle$ is an eigenfunction of H_0

$$H_0|n\rangle=\epsilon_n|n\rangle \tag{2.3a}$$

with total oscillator quanta n. All other quantum numbers (such as spin, isospin, orbital angular momentum, etc.) needed to specify this antisym-

metric function are implied, but not written explicitly. The sum in Eq. (2.3) is taken only up to some maximum number of oscillator quanta N_0. If N_0 were taken to be infinite, we would have an exact formulation of the problem.

The functions χ_{ij} will be written as

$$|\chi_{ij}\rangle = \sum_{\alpha > N_0} |\alpha(ij)\rangle\langle\alpha|\Psi\rangle , \tag{2.4}$$

These states $|\alpha(ij)\rangle$ are also eigenfunctions of H_0

$$H_0|\alpha(ij)\rangle = \epsilon_\alpha|\alpha(ij)\rangle \tag{2.4a}$$

with total oscillator quantum number α (all other quantum numbers are implied). The difference $|n\rangle$ and $|\alpha(ij)\rangle$ is that the latter are not totally antisymmetric. $|\alpha(ij)\rangle$ is actually a simpler basis vector composed of a product of an antisymmetric function for particles i and j and a second function antisymmetric and all other particles, e.g.,

$$\langle\vec{q}_1\cdots\vec{q}_A|\alpha(1,2)\rangle = \langle\vec{q}_1\vec{q}_2|\alpha_1\rangle\langle\vec{q}_3\cdots\vec{q}_A|\alpha_2\rangle , \tag{2.4b}$$

$(\alpha_1 + \alpha_2 = \alpha)$, so that there is no symmetry restriction implied above between particle 1 (or 2) and particles 3 to A. Note that the ij designation is not needed in $\langle\alpha|\Psi\rangle$ because all pairs of nucleons are equivalent.

Using this prescription for the wave function and multiplying Eq. (2.1) from the left by $\langle k|$, one finds

$$(E-\epsilon_k)\langle k|\Psi\rangle = \langle k|V|\Psi\rangle \cong \langle k|V|\Phi\rangle + \sum_{i<j}\langle k|v_{ij}|\chi_{ij}\rangle . \tag{2.5}$$

In the second line of Eq. (2.5) one neglects terms like $\langle k|v_{ij}|\chi_{i'j'}\rangle$ with $ij \neq i'j'$. This approximation will be made consistently in the remainder of this presentation and discussion is left until the end of this section. Multiplying Eq. (2.1) by $\langle\alpha(ij)|$, one obtains [for consistency with the previous approximation one must consider the $|\alpha(ij)\rangle$ to be orthogonal, $\langle\alpha(ij)|\alpha(i'j')\rangle = \delta_{ii'}\delta_{jj'}$]:

$$\begin{aligned}(E-\epsilon_\alpha)\langle\alpha|\Psi\rangle &\cong \langle\alpha(ij)|v_{ij}|\Phi\rangle + \langle\alpha(ij)|v_{ij}|\chi_{ij}\rangle \\ &\cong \sum_n \langle\alpha(ij)|v_{ij}|n\rangle\langle n|\Psi\rangle \\ &\quad + \sum_{\alpha'}\langle\alpha(ij)|v_{ij}|\alpha'(ij)\rangle\langle\alpha'|\Psi\rangle .\end{aligned} \tag{2.6}$$

Multiplying Eq. (2.1) by $\langle\Phi|$, and imposing the normalization condition

$$\langle\Phi|\Phi\rangle = \sum_{n=0}^{N_0}\langle\Psi|n\rangle\langle n|\Psi\rangle = 1, \tag{2.7}$$

the energy is given by

$$\begin{aligned}E &= \langle\Phi|H_0+V|\Psi\rangle \\ &\cong \langle\Phi|H_0+V|\Phi\rangle + \sum_{i<j}\sum_\alpha\langle\Phi|v_{ij}|\alpha(ij)\rangle\langle\alpha|\Psi\rangle .\end{aligned} \tag{2.8}$$

Equation (2.5) can be rewritten in a more convenient form:

$$\begin{aligned}(E-\epsilon_n)\langle n|\Psi\rangle &= \sum_{n'}\langle n|V|n'\rangle\langle n'|\Psi\rangle \\ &\quad + \sum_{i<j}\sum_\alpha\langle n|v_{ij}|\alpha(ij)\rangle\langle\alpha|\Psi\rangle .\end{aligned} \tag{2.9}$$

Equations (2.6) through (2.9) form the basic relationships of the method to be tested in this paper. Mathematical solutions are elementary since Eqs. (2.6) and (2.9) form a linear set of equations in $\langle n|\Phi\rangle$ and $\langle\alpha|\Psi\rangle$ which must be solved self-consistently with the expression for the energy in Eq. (2.8), retaining the normalization condition in Eq. (2.7).

To understand the relationship with other methods it is instructive to introduce the two-body g matrix

$$g_{ij} \equiv v_{ij} + v_{ij}\left(\frac{Q_{ij}}{e}\right)g_{ij} , \tag{2.10}$$

with

$$\frac{Q_{ij}}{e} \equiv \sum_{\alpha > N_0}\frac{|\alpha(ij)\rangle\langle\alpha(ij)|}{E-\epsilon_\alpha} . \tag{2.11}$$

Equation (2.6) is easily seen to be equivalent to the Bethe-Goldstone equation

$$(E-H_0)|\chi_{ij}\rangle = v_{ij}|\Phi\rangle + Q_{ij}v_{ij}|\chi_{ij}\rangle . \tag{2.12}$$

Equations (2.8) and (2.9) can be reexpressed in terms of the g matrix

$$(E-\epsilon_n)\langle n|\Psi\rangle = \langle n|\sum_{i<j}g_{ij}|\Phi\rangle , \tag{2.13}$$

$$E = \langle\Phi|H_0 + \sum_{i<j}g_{ij}|\Phi\rangle . \tag{2.14}$$

Equations (2.13) and (2.14) take the *form* of a variational calculation in which g_{ij} has replaced the interaction v_{ij}. Of course this replacement results in the loss of the variational property of the calculation, so that E is not necessarily an upper bound on the true eigenvalue. What one actually has above is an "extended g-matrix formalism." The "extension" is in the sense that the first-order wave function Φ can be a linear combination of oscillator states rather than a single

determinant. Equations (2.13) and (2.14) [or alternatively, Eqs. (2.6) through (2.9)] yield a simple prescription for the linear combination through solution for the $\langle n|\Phi\rangle$. In the present form the method is as easy to apply to degenerate as well as nondegenerate first-order configurations.[9,10]

The formalism described above is fully equivalent to solutions of the Bethe-Faddeev equation in a truncated oscillator basis.[5,6] One should note that although the same results will be obtained, intermediate definitions are different. In particular the Pauli operator (Q_{ij}) is defined in Eq. (2.11) to include oscillator states only with $\alpha > N_0$. In solving the Bethe-Faddeev equations one includes states of lower values of α, and then directly excludes redundant diagrams of the type

$$\left\langle 0\left| g_{12}\frac{Q}{e}g_{12}\right|0\right\rangle.$$

This latter procedure is more useful when one solves the Bethe-Goldstone equation in configuration[1-3] (or momentum) space. In this paper, however, we will deal with a truncated set of vectors in a matrix representation,[11] so that the greatest mathematical convenience is provided by Eqs. (2.6) through (2.9). These, in turn correspond to the g matrix defined by Eqs. (2.10) and (2.11). If Φ consists of only a single function (with minimum oscillator quanta) one has the usual g-matrix formalism (with starting energy E).

There are two approximations inherent in the above formalism:

(i) The vectors $|\alpha(ij)\rangle$ are not antisymmetric with respect to interchange of *all* pairs of nucleons.

(ii) Only the nucleons i and j are active in $|\alpha(ij)\rangle$, so that one neglects cross terms like $\langle\alpha(12)|v_{13}|\alpha'(12)\rangle$.

Both approximations are directly related to truncating the sum n at N_0 in Eq. (2.3). The errors expected from either approximation individually may be expected to be substantial. It has been demonstrated[6] that these errors cancel each other very sharply as N_0 increases. The proof, however, depends on perturbation theory, and may break down when the perturbation expansion fails to converge.

In addition, this cancelation must depend quantitatively on the two-body interaction which is employed. The purpose of this paper is to make quantitative tests of the accuracy for interactions of a realistic character.

III. TENSOR FORCES AND $-U$ INSERTIONS

An appropriate form for the intrinsic nuclear Hamiltonian is obtained by taking

$$H_0 = \tfrac{1}{2}\hbar\omega\sum_i (p_i^2+q_i^2) - H_{\text{c.m.}}, \tag{3.1}$$

$$V = v^N - U, \tag{3.1a}$$

where

$$U = \tfrac{1}{2}\hbar\omega\left(\sum_i \tilde{q}_i - A^{-1}\sum_j \tilde{q}_j\right)^2$$

$$= \left(\frac{\hbar\omega}{2A}\right)\sum_{i<j} q_{ij}^2 \tag{3.1b}$$

and v^N is the nucleon-nucleon interaction operator.

There are three outstanding possible sources of difficulty in attempting accurate solutions for the energy eigenvalue, when realistic nuclear interactions are used:

(i) The nuclear force retains a strong short-range component, which forces the wave function toward zero at small nucleon-nucleon separations.

(ii) The tensor component of the nuclear force is quite strong, and of comparatively long range. This may cause substantial three-body correlations.

(iii) The matrix elements of U are large and increase in magnitude as the number of oscillator quanta increases. These terms are curious in that they arise from the way the problem has been formulated rather than from the physical nature of the nuclear forces. One uses an oscillator basis in this problem primarily because of their analytical properties (particularly the separability of the center of mass). The tail of the oscillator orbitals is Gaussian rather than the expected exponential character. The $-U$ term in Eq. (3.1a) corrects the shape of the orbitals as it mixes in higher oscillator configurations, and may give rise to large three-body correlations due to the divergent character of its matrix elements in a perturbation expansion.

In this section we shall perform a convergence test by calculating ^{3}H with the Sussex interaction.[12] This interaction should present us with all facets of a realistic nuclear force except for the short range repulsive core, which will be examined in Sec. IV of this paper. This interaction is convenient mainly because it is in the form of a set of oscillator matrix elements, and it has already been demonstrated[13,14] that it yields a reasonable binding energy for 0s-shell nuclei when only a modest number of oscillator quanta are allowed to be excited in the calculation.

Oscillator basis states for ^{3}H which are totally antisymmetric and properly invariant under translations are constructed employing the Jacobi coordinates

TABLE I. Calculations of the energy eigenvalue of ^{3}H with the Sussex matrix elements [at $b = 1.6 \times 10^{-13}$ cm]. All results were obtained with $N = 8$, and propagator e^{-1}.

N_0	0	2	4	6	8
$-E$ (MeV)	3.49	3.68	4.31	4.63	4.67
% error	25%	21%	8%	1%	...

$$\vec{x} = (2)^{-1/2}(\vec{q}_1 - \vec{q}_2)\,, \tag{3.2a}$$

$$\vec{y} = (6)^{-1/2}(\vec{q}_1 + \vec{q}_2 - 2\vec{q}_3). \tag{3.2b}$$

The prescription for this construction has been previously given in detail by Moshinsky[15,16] and his collaborators. The basis states $|\alpha(ij)\rangle$ are trivial to construct:

$$\langle \vec{q}_1\vec{q}_2\vec{q}_3 \,|\, \alpha(12)\rangle = \langle \vec{x} \,|\, nlsj\tau\tau_3\rangle \langle \vec{y} \,|\, n'l's'j'\tau'\tau_3'\rangle. \tag{3.3}$$

Vector coupling of j and j' to $\frac{1}{2}$ (and τ, τ' to $\frac{1}{2}$) is implied above. It should also be noted that these functions are translationally invariant, and antisymmetric under interchange of particles 1 and 2.

Table I presents a straightforward example with the Sussex matrix elements at $b = 1.6 \times 10^{-13}$ cm. All results in the table were obtained with $N = 8$ as the maximum number of quanta included in the g-matrix computation, while N_0 is defined as the maximum number of quanta in the sum on the right-hand side of Eq. (2.3). When $N_0 = 8$, one has a completely variational calculation including all S and D states up to eight oscillator quanta. The eigenvalue obtained ($E = -4.67$ MeV) seems to be in reasonable agreement with the value $E = -4.41$ MeV obtained by Jackson and Elliott[14] [with $N = 8$, $b = 1.5 \times 10^{-13}$ cm], with a variational calculation including only certain selected [3]S and [21]D states.

The value $E = -4.67$ MeV may then be regarded as a "precise" result in Table I, just for purposes of comparison. If the g-matrix calculations presented there worked perfectly, they could do no better than reproduce this value for the energy. What one actually sees can be labeled no better than a moderate success for the g-matrix method. For $N_0 = 0$, one is a bit more than 1 MeV (25%) short of the full binding energy. As N_0 increases, one steadily approaches the precise result, with the major correction coming at $N_0 = 4$.

As one performs this calculation, the major source of error in the g matrix becomes very clear. The primary difference between the energy matrix generated by Eqs. (2.6), (2.8), and (2.9) and the actual energy matrix of the variational method lies in the diagonal terms; or in other words the energy denominators of the propagator from the g matrix. These terms have long been suspect,[1,17,18] and relate to the well known problem of selecting an appropriate single-particle energy in the excited particle states.

The diagonal term in Eq. (2.9) (that is the coefficient of $\langle n \,|\, \psi\rangle$) is

$$E - \epsilon_n - \langle n \,|\, V \,|\, n\rangle\,, \tag{3.4}$$

while the diagonal term of Eq. (2.6) (the coefficient of $\langle \alpha \,|\, \psi\rangle$) is

$$E - \epsilon_\alpha - \langle \alpha(ij) \,|\, v_{ij} \,|\, \alpha(ij)\rangle\,. \tag{3.5}$$

There is no difference in replacing ϵ_n by ϵ_α, but the difference between $\langle n \,|\, V \,|\, n\rangle$ and $\langle \alpha(ij) \,|\, v_{ij} \,|\, \alpha(ij)\rangle$ is very great. The V interaction defined by Eq. (3.1a) retains the $-U$ term, which corrects for using a harmonic oscillator potential in H_0. These $-U$ insertions increase in magnitude in direct proportion to the number of oscillator quanta; and, in effect, nearly cut the effective value of ϵ_n in half. But in the particle states (α) one is including only one single-particle insertion for the triton instead of three, and consequently one calculates the g matrix with energy denominators in the propagator which are far too large in magnitude. This constitutes the primary error made in the g-matrix calculations of Table I.

The error is easily corrected. The energy denominator used for the calculation of Table I could be written

$$\langle \alpha \,|\, e^{-1} \,|\, \alpha\rangle = (E - E_\alpha)^{-1}$$
$$= (E - \langle \alpha \,|\, H_{0x} + H_{0y} \,|\, \alpha\rangle)^{-1}\,. \tag{3.6}$$

The $\langle \alpha(ij) \,|\, v_{ij} \,|\, \alpha(ij)\rangle$ terms are included in the two-body interaction but not the propagator. H_{0x} and H_{0y} are the components of $H_0 = H_{0x} + H_{0y}$, corresponding to the Jacobi coordinates of Eqs. (3.2a) and (3.2b). Now to correct the propagator for the two additional $-U_{ij}$ insertions one simply replaces the harmonic oscillator potential insertions in the energy denominator equal by zero for the inactive pairs of nucleons. The clearest way to construct this is to define a new propagator simply as

$$\langle \alpha(12) \,|\, (e')^{-1} \,|\, \alpha(12)\rangle$$
$$= [E - \langle \alpha(12) \,|\, H_{0x} + H_{0y} - U_{13} - U_{23} \,|\, \alpha(12)\rangle]^{-1}\,. \tag{3.7}$$

The two propagators e and e' are compared in Table II. All g-matrix calculations in this table were performed with $N_0 = 0$. The g-matrix calculations are then displayed where only a certain

TABLE II. Calculations of the energy eigenvalue of ^{3}H (in MeV) with the Sussex matrix elements [at $b = 1.6 \times 10^{-13}$ cm]. Comparison is made between the variational method, the g-matrix method with two different propagators defined in the text (all with $N_0 = 0$), and two varieties of second-order perturbation theory,[a] as a function of N.

Method	N	2	4	6	8
Variational		-1.42	-3.61	-4.29	-4.67
g matrix: e'		-1.51	-3.34	-4.09	-4.64
e		-1.05	-2.38	-3.04	-3.49
second order perturbation theory: I		-1.95	-4.00	-5.05	-5.70
II		-1.56	-3.54	-4.55	-5.19

[a] Perturbation method I utilizes the intermediate states $|\alpha(ij)>$, while method II employs the properly antisymmetric intermediate states $|n>$.

maximum number of oscillator quanta N are included in the entire calculation; and at each stage are to be compared with a variational calculation performed with the same number of oscillator quanta. The propagator with e' is seen to yield a much improved accuracy over the propagator with e. In no example was agreement poorer than a 6% error, and this was for $N = 2$ where one expects maximal errors for the method. At $N = 8$ the new propagator yields agreement to within a 1% error with the variational result.

Perturbation theory results are also included in Table II for comparison. There are two ways to do the perturbation calculation. One is to use the $|\alpha(ij)\rangle$ as the intermediate states

$$E_{\mathrm{I}} = \epsilon_0 + \langle 0|V|0\rangle + \sum_{\alpha, i<j} \frac{|\langle 0|v_{ij}|\alpha(ij)\rangle|^2}{\epsilon_0 - \epsilon_\alpha}, \tag{3.8}$$

the other to use the fully antisymmetric states $|n\rangle$

$$E_{\mathrm{II}} = \epsilon_0 + \langle 0|V|0\rangle + \sum_{n\neq 0} \frac{|\langle 0|V|n\rangle|^2}{\epsilon_0 - \epsilon_n}. \tag{3.9}$$

In both cases the Rayleigh-Schrödinger perturbation method was applied up to second order and all states up to the maximum number of oscillator quanta (N) were included.

Perturbation method I (using $|\alpha(ij)\rangle$ yields uniformly mediocre agreement with the variational calculation. Method II (using $|n\rangle$) seems to do considerably better. Note, however, that method II grows poorer for larger values of N. The agreement of at lower values of N is actually spurious. The higher order perturbation corrections are attractive for the central interaction and repulsive for the tensor force. At low N the resulting cancellation improves the overall accuracy. At larger N, however, the contributions of the tensor force become much more important than those of the central (central forces yield very little additional energy for $N>4$), and perturbation theory will badly overestimate the binding energy.

IV. SHORT-RANGE REPULSION

The use of the Sussex interaction in Sec. III should cover all difficulties encountered with realistic nuclear forces, except for the strong short-range repulsion. This latter component is certainly lacking from the Sussex matrix elements, and we shall perform a separate test on it in this section. One could just add a short-range term to the Sussex interaction. Since there seems to be no way to fit such a term either to scattering or bound state data without diminishing agreement with experiment, such a procedure would not seem to be advisable. Besides, some interesting information will be obtained by isolating the repulsive core.

The example chosen for illustration is one of three nucleons in an oscillator well

$$H_0 = \tfrac{1}{2}\hbar\omega \sum_{i=1}^{3} (p_i^2 + q_i^2) - H_{\mathrm{c.m.}}, \tag{4.1}$$

perturbed by a repulsive δ-function interaction

$$V = V_0 \sum_{i<j} \delta(\vec{q}_i - \vec{q}_j). \tag{4.2}$$

There are several reasons for selecting the δ-function interaction. First, it has a simple analytic character with regard to calculations done in this paper. Matrix elements of the two-body interaction, in oscillator states of the relative motion $\vec{x}$ [defined in Eq. (3.2a)], may be expressed in terms of the Talmi integrals[16,19]

$$\langle \varphi_{nl}(x)|v_{12}(x)|\varphi_{n'l'}(x)\rangle = \sum_p B(nl, n'l', p) I_p, \tag{4.3}$$

where

$$I_p = 2[\Gamma(p+\tfrac{3}{2})]^{-1} \int_0^\infty v_{12} x^{2p+2} \exp(-x^2) dx, \tag{4.4}$$

and the coefficients $B(nl, n'l', p)$ are easily derived in closed form.[16] For a δ-function interaction, only terms with $p = l = l' = 0$ are needed, and one has

$$B(n0, n'0, 0) = 2^{-(n+n')}(n!n'!)^{-1}[(2n+1)!(2n'+1)!]^{1/2}. \tag{4.5}$$

The main advantage is that the properties of the interaction are summarized in just one parameter, the Talmi integral I_0. All other Talmi integrals are zero.

The second reason for choosing the δ function

is that all orders of perturbation theory above first order are infinite. Thus one can test the convergence of the g-matrix method for a case where perturbation theory will clearly not be convergent.

Of course the δ-function interaction is just a model of the nuclear repulsive core. One could select a repulsive Gaussian

$$v_{12} = V_0(1+\alpha^2)^{3/2}\exp(-\alpha^2 x^2) \tag{4.6}$$

so that

$$I_{n+1} = (1+\alpha^2)^{-1} I_n . \tag{4.6a}$$

For a half width $\alpha > 7$ one would obtain approximately the same results in the calculations presented in this section. The only significant property of the δ function used here is that it acts only in relative S states with all Talmi integrals other than I_0 negligible.

Some sample calculations are shown in Table III. Owing to the independence of the Hamiltonian on spin and isospin, only the orbitally symmetric [3] S states are needed in the variational calculations in this table. The g-matrix calculations in this table are all performed with $N_0 = 0$. One can then directly compare the g-matrix calculation, done with a maximum number of N oscillator quanta, with a variational bound in the corresponding vector space. Second-order perturbation calculations using the $|\alpha(ij)\rangle$ (method I) and $|n\rangle$ (method II) are also presented for comparision. In order to give a clearer picture of the various methods, only the energy shift due to configuration mixing

$$\Delta E = E - 3\hbar\omega - 3I_0 \tag{4.7}$$

is tabulated.

For $I_0 = \frac{1}{3}\hbar\omega$, the g-matrix calculation reproduces the variational result with remarkable accuracy. Poorest agreement is found at the lowest values of N, as predicted. Perturbation theory, on the other hand, becomes progressively worse as N increases One should be reminded that either second-order perturbation method will behave like $\sum N^{-1/2}$ for large N, and this is not a convergent series.

For $I_0 = \hbar\omega$, agreement between the g-matrix and the variational method is not as good. At $N = 2$ the g matrix yields a 20% error. As N increases the accuracy of the g matrix improves rapidly; yielding only a 5% error at $N = 8$. Perturbation results are now absurd. One has an obvious bound $\Delta E > -3\hbar\omega$, and this limit is already passed at $N = 2$ by perturbation method II.

The case with $I_0 = \hbar\omega$ is interesting because now we can see how extending the basis (N_0) will improve the approximate eigenvalue. Table IV displays ΔE as a function of N_0 and N. The diagonal terms of this table ($N = N_0$) represents variational calculations. As one reads down any column of this table one sees how the g-matrix calculation approaches the variational result as the basis is extended. Note that the change in ΔE when one goes from $N_0 = 0$ to $N_0 = 2$ appears to always be at least indicative of the magnitude of the error at $N_0 = 0$, and that an accuracy comparable to the case where $I_0 = \frac{1}{3}\hbar\omega$ is generally obtained at least by $N_0 = 4$.

How does the strength of the repulsive interaction tested here compare to that in realistic nuclear forces? Perhaps the best basis for comparison is to examine the wound integral:

TABLE III. Energy shifts, $\Delta E = E - 3\hbar\omega - 3I_0$, for the δ-function interaction with strengths $I_0 = \frac{1}{3}\hbar\omega$ and $I_0 = \hbar\omega$. Values of ΔE calculated by the variational method, g-matrix method (with $N_0 = 0$), and second-order perturbation theory are presented for comparison. N is the maximum number of oscillator quanta allowed in each computation, and ΔE is tabulated in units of $\hbar\omega$.

N	Variational	g matrix	Perturbation method I	Perturbation method II
		$I_0 = \frac{1}{3}\hbar\omega$ ($\Delta E = E - 4\hbar\omega$).		
		$\Delta E/\hbar\omega$		
2	-0.30	-0.28	-0.25	-0.37
4	-0.36	-0.37	-0.41	-0.55
6	-0.41	-0.40	-0.53	-0.68
8	-0.46	-0.45	-0.63	-0.78
		$I_0 = \hbar\omega$ ($\Delta E = E - 6\hbar\omega$)		
		$\Delta E/\hbar\omega$		
2	-1.58	-1.89	-2.25	-3.37
4	-1.95	-2.07	-3.66	-4.97
6	-2.02	-2.13	-4.75	-6.09
8	-2.08	-2.18	-5.67	-7.02

TABLE IV. Energy shifts $\Delta E = E - 3\hbar\omega - 3I_0$, for the δ-function interaction with $I_0 = \hbar\omega$. Calculations are performed with the g-matrix method in an extended basis [using Eqs. (2.6), (2.7), (2.8), and (2.9)], as a function of N and N_0.

		$\Delta E/\hbar\omega$				
N_0	N	0	2	4	6	8
0		0	-1.89	-2.07	-2.13	-2.18
2			-1.58	-1.95	-2.07	-2.14
4				-1.95	-2.03	-2.11
6					-2.02	-2.09
8						-2.08

$$\left\langle \Phi \left| \frac{-\partial g}{\partial E} \right| \Phi \right\rangle = \sum_{\alpha} |\langle \Psi | \alpha \rangle|^2$$
$$= 0.04 \quad \text{for } I_0 = \tfrac{1}{3}\hbar\omega$$
$$= 0.10 \quad \text{for } I_0 = \hbar\omega, \tag{4.8}$$

where the quoted numbers correspond to $N_0 = 0$. For realistic interactions one normally finds a wound integral on the order of 0.02 in the $^1S_0$ state,[18,20] so that the case $I_0 = \frac{1}{3}\hbar\omega$ appears to be a reasonably strong interaction. An alternative way to judge the strength at $I_0 = \frac{1}{3}\hbar\omega$ is to note that it will yield nearly identical results (to better than 1%) to a repulsive Gaussian [Eq. (4.6)] with range parameter 0.2×10^{-13} cm and maximum height ~2830 MeV, if b is chosen to be $1.6(10^{-13})$ cm.

It is also interesting to note that

$$\langle \Phi | -\hbar\omega \frac{\partial^2 g}{\partial E^2} | \Phi \rangle = 0.03 \quad \text{for } I_0 = \tfrac{1}{3}\hbar\omega$$
$$= 0.16 \quad \text{for } I_0 = \hbar\omega. \tag{4.9}$$

The numbers in Eqs. (4.8) and (4.9) seem to bear out the idea[6] that a large value for $\partial^2 g/\partial E^2$ indicates poorer convergence. A precise quantitative criterion relating the magnitude of the second derivative to the size of the error in the energy is unfortunately lacking.

V. CONCLUSIONS

Comparison of the g-matrix and variational calculations, both performed in a basis with an identical maximum number of oscillator quanta, demonstrates that the g-matrix procedure is capable of a remarkably high degree of accuracy. The most enlightening way to obtain a general idea of how much accuracy can be anticipated in a particular problem is to discuss where the difficulties can be expected.

In all the examples tested in this investigation the difficulties appeared to originate from the diagonal terms in Eq. (2.6). This has already been emphasized for the Sussex interaction, where a simple alteration of the g-matrix propagator corrected the difficulty. A similar problem arises with the δ-function interaction. It is not so severe, but neither is it so easily corrected. The point is that

$$\langle \alpha | v_{ij} | \alpha \rangle \tag{5.1}$$

[appearing in Eq. (2.6)] is simply not nearly as large as

$$\langle n | V | n \rangle \tag{5.2}$$

[appearing in Eq. (2.9)], because in the latter the multiparticle effects are coherent and the rearrangement energy is also included. The difference is quite substantial at $N = 2$, as one can clearly see in Table IV. The error diminishes rapidly for increasing N, and appears to be very moderate for a realistic strength of the interaction. It will tend to be more important, however, in a heavier nucleus.

There are several remedies for this deficiency when it becomes sufficiently important. Becker, MacKellar, and Morris[17] introduce an additional parameter into the propagator which produces a uniform displacement in all diagonal terms. Although this will improve the average value of the energy denominators, a detailed comparison of Eqs. (2.6) and (2.9) shows that the energy shift should be variable depending on the state. A better prescription, in a fully Brueckner ized formalism, would be to employ the partial occupation probabilities introduced by Brandow.[9]

There is a straightforward way to correct the energy denominators within the context of the procedures employed in this paper. Simply extend the basis (increase N_0). Since the discrepancies diminish rapidly as a function of N, it is unlikely that one will be forced to make N_0 very large. Of course, the value of N_0 required will depend on the interaction one is working with, the physical system under investigation, and the accuracy desired.

In any case, it appears that one should extend the basis at least to $N_0 = 4$ as a check on the accuracy of the approximations. In all examples tested in this investigation, such a check gave a clear indication of the error incurred by truncating to $N_0 = 0$, and if H_0 and V are partitioned in an appropriate manner, the results at $N_0 \leq 4$ were quite accurate. It is also quite likely that such a procedure will reveal a prescription for the energy denominators that will yield satisfactory results at $N_0 = 0$, as in the example of Sec. III.

Extension of the basis will be limited in practice by the dimension of the vector space defined by the states $|n\rangle$ in Eq. (2.3). In the very light nuclei ($A \leq 4$) this presents little problem. Even in nuclei as heavy as ^{16}O this appears to be feasible. Application to heavier nuclei will probably depend on one's ingenuity in making a further truncation of the basis. Reasonable possibilities for such truncations are well known. For example, in ^3H one could neglect all P states and [111] S states without modifying the results significantly.[14] Even the [21] S states can be suppressed without serious complications. Since such truncations were not found to be needed in the present work, however, we will not discuss them in detail here.

As a further illustration of the use of the formalism, the g-matrix calculation for the Sussex inter-

action was extended to $N=14$, using the energy denominator e' defined by Eq. (3.7). At $N_0=0$, the eigenvalue for ^{3}H was estimated to be −5.31 MeV. Extension of the basis to $N_0=4$ increased the binding energy by only 0.03 MeV. Clearly one has not yet reached convergence as a function of N. Important matrix elements needed to increase N are lacking. In addition, one is now approaching the point where π-meson production is important in analysis of the scattering data, and relativistic effects may become more significant.

The simple g-matrix calculation is adequate to demonstrate that the Sussex interaction yields a reasonable binding energy for the triton, but that more work must be done to obtain quantitative agreement with experiment. In addition, since the discrepancy with the experimental value is about 3 MeV, a more exact (and much more difficult) variational calculation is not warranted.

Are there any restrictions on the two-body force one employs in this method? If the perturbation expansion for the interaction converges, then this method must converge also. This is a sufficient condition, however, and clearly not a necessary one. Application to the δ-function interaction was quite successful, and this interaction leads to a divergent perturbation series. The only criterion available here is a detailed comparison with the variational method, and this may not be practical for heavy nuclei. A rigorous necessary condition does not appear to be yet available in a simple form.

Three-body forces may also be important in determining the triton binding energy.[21] One important advantage of the extended g-matrix formalism is the straightforward way in which many-body forces can be incorporated into the calculation. No effort was made to include them in the present investigation, however, simply because of the obvious uncertainties in the details of their nature.

The author plans to extend this work to calculations on ^{4}He and ^{16}O in the near future. The major problems to be considered in these calculations are the connection with the Brueckner-Bethe-Goldstone energy denominators, and additional truncations of the basis.

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