Shell-Model Analysis for Brueckner Calculations in Light Nuclei*

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Brueckner self-consistent calculations are performed for ^{16}O, ^{3}H, and ^{4}He nuclei with various modern hard-core interactions. Elements of the G matrix are calculated by the reference-spectrum method, while $Q-1$ corrections are made by matrix inversion in the proper single-particle space. Thus, it is not assumed that Q commutes with the center-of-mass motion. The prescription for selecting the appropriate spectrum of single-particle excited states is investigated by comparing results of the Brueckner method with other calculations. These comparisons indicate that the particle spectrum should be left unperturbed. One then finds that the Hamada-Johnston, Yale, and Reid (hard-core) interactions yield about one half the binding energy of ^{16}O. The calculated results are dissected into shell-model components. This analysis indicates that the short-range part of the hard-core interaction is too strongly repulsive.

I. INTRODUCTION

The success of the Brueckner-Bethe-Goldstone method in calculating the properties of nuclear matter[1,2] has encouraged many applications to finite nuclei[3] over the past decade.[4] These applications usually are based on the solution of the Bethe-Goldstone equation

$$\psi(\vec{x}_1,\vec{x}_2)=\phi(\vec{x}_1,\vec{x}_2)+\frac{Q}{W-H_0}v_{12}\psi(\vec{x}_1,\vec{x}_2), \tag{1.1}$$

where ψ is the correlated two-body wave function, ϕ is the unperturbed shell-model wave function (normally taken as harmonic-oscillator orbitals), Q is the Pauli operator which forbids the scattering of nucleons into occupied orbitals, and v_{12} is the nucleon-nucleon interaction. H_0 is the (unperturbed) single-particle (shell-model) Hamiltonian and W is the starting energy, both of which will be defined more closely later.

Elements of the nuclear G matrix

$$G=v_{12}+v_{12}\frac{Q}{W-H_0}G \tag{1.2}$$

are then generated through the relationship

$$\langle\phi|\,G\,|\,\phi\rangle=\langle\phi|\,v_{12}\,|\,\psi\rangle. \tag{1.3}$$

Solution of Eq. (1.1) for ψ is often effected by the reference-spectrum method of Bethe, Brandow, and Petschek.[5] The popularity of this method is derived from two basic points:
(1) It is relatively easy to implement, especially when high speed computers are available.
(2) When applied with all of its refinements, it is capable of unlimited accuracy.
In preliminary calculations[6] we found this method to be significantly more accurate than the separation method of Moszkowski and Scott. Consequently it is the method employed in this paper.

To solve Eq. (1.1) one first sets Q equal to unity obtaining

$$(W-H_0)(\psi-\phi)=v_{12}\psi. \tag{1.4}$$

The methods for solving this linear differential equation are well known[3] and have been reviewed elsewhere. We shall not attempt to justify setting $Q=1$, for indeed it is a poor approximation. It is, however, easy and straightforward to correct this point. First define the approximate reference-spectrum matrix elements by

$$G_R=v_{12}+v_{12}\frac{1}{W-H_0}G_R. \tag{1.5}$$

Comparison of Eqs. (1.2) and (1.5) yields (after a little algebra)[5]

$$G=G_R+G_R^{\dagger}\frac{Q-1}{W-H_0}G. \tag{1.6}$$

The right-hand side of Eq. (1.6) may be expanded out iteratively into an infinite series

$$G=\sum_{n=0}^{\infty}G_R(bG_R)^n, \tag{1.7a}$$

where

$$b=\frac{Q-1}{W-H_0}, \tag{1.7b}$$

and then summed by the usual rule for an harmonic series:

$$G=G_R\frac{1}{1-bG_R}. \tag{1.8}$$

Equation (1.8) appears quite formidable, since b and G_R are both complicated operators. Kohler and McCarthy,[7] however, have shown that solutions are easily found in matrix form. First set

up the matrices $\langle m|\, b\,|\, n\rangle$ and $\langle m|\, G_R|\, n\rangle$. Then one has

$$\langle n|\, 1 - bG_R|\, m\rangle = \delta_{nm} - \sum_k \langle n|\, b\,|\, k\rangle\langle k|\, G_R|\, m\rangle . \quad (1.9)$$

The matrix $\langle n|\, 1 - bG_R|\, m\rangle$ can then be inverted and combined into Eq. (1.8) to give

$$\langle n|\, G|\, m\rangle = \sum_k \langle n|\, G_R|\, k\rangle\langle k|\, (1 - bG_R)^{-1}|\, m\rangle , \quad (1.10)$$

which provides the matrix elements of G, properly corrected for the Pauli principle. The only operations needed are matrix inversion and multiplication.

A second problem in the application of the reference-spectrum method lies in the selection of H_0, which determines the spectrum of excited "particle" states (hence the title of this procedure). This selection is of paramount importance, as it can strongly influence the outcome of the calculation.[3,8-10] A dominant consideration for finite nuclei is that the two-nucleon Hamiltonian

$$H_0(1, 2) = H_0(1) + H_0(2) \quad (1.11)$$

must be separable into relative and center-of-mass coordinates:

$$H_0(1, 2) = H_0(x, p) + H_0(X, P) , \quad (1.12a)$$

where

$$\vec{x} = \vec{x}_1 - \vec{x}_2 , \quad (1.12b)$$

$$\vec{X} = \tfrac{1}{2}(\vec{x}_1 + \vec{x}_2) . \quad (1.12c)$$

Otherwise, one would be confronted by the three-body problem.

This narrows the selection to either the free-particle propagator

$$T = p^2/2m + \Delta \quad (1.13)$$

or to the harmonic oscillator

$$H_{\rm osc} = p^2/2m + \tfrac{1}{2}kx^2 + \Delta . \quad (1.14)$$

Δ is a constant representing a uniform displacement of the excited states. The unperturbed shell-model functions ϕ are universally taken to be oscillator orbitals in finite nuclei, because of their separability under the Brody-Moshinsky[11] transformation. Consistency would then appear to dictate choosing $H_{\rm osc}$ in the propagator.

Baranger,[3] however, has emphasized that this is not clearly the case. If one defines

$$H_0 = T + U , \quad (1.15)$$

where U is the shell-model (single-particle) potential, then

$$H = H_0 + \sum_{i<j} v_{ij} - U . \quad (1.16)$$

One then sees that the usual Feynman-Goldstone ladder diagram should contain $-U$ insertions in the particle lines. These $-U$ insertions are compensated for if one uses a G matrix defined by[3]

$$G_{ij} = v_{ij} + v_{ij}\frac{Q}{W - QTQ}G_{ij} , \quad (1.17a)$$

where the appearance of Q in the denominator insures that the (excited) particle states are orthogonal to the (occupied) hole states. Brandow,[12] however, has argued that the QTQ term in the denominator should be replaced by T, as is usually done in practice.

In this paper we report primarily calculations performed with the plane-wave [Eq. (1.13)] propagator

$$G_R = v_{12} + v_{12}\frac{1}{W - T - \Delta}G_R . \quad (1.17b)$$

It remains, however, to determine the appropriate displacement (Δ) of the particle spectrum. This determination is critical, since the binding energy per nucleon is found to increase by about 1 MeV each time Δ is reduced by 10 MeV.[3,8,9] Two different assumptions concerning the value of Δ have received attention (see Ref. 3 for a concise critical review of this point). The first is to set $\Delta = 0$, leaving the single-particle spectrum unperturbed. These calculations yield binding of only 3 or 4 MeV per nucleon in ^{16}O, when realistic interactions are used. The second method takes Δ of the order of -50 to -70 MeV in ^{16}O. The logic behind this is that the energy of the occupied $1s$ and $1p$ orbitals is calculated self-consistently, and found to be displaced below their unperturbed positions by roughly this amount. Why not displace all levels accordingly? These calculations[8] yield 7 to 8 MeV per nucleon binding in ^{16}O, which is close to the experimental value.

The difference arises out of the fact that, within the content of a first-order G-matrix calculation, there is no criterion for specifying Δ. Such a criterion could be established through rigorous evaluation of the three-body terms. This would be equivalent to solving the Faddeev[13] equations for ^{16}O, a formidable task which to our knowledge has never been attempted.

An alternative procedure for estimating the appropriate value of Δ would be to compare G-matrix calculations with other methods for equivalent problems. In addition, we shall demonstrate that unrealistic values of Δ can be rejected by performing a shell-model analysis on the calculation.

II. PROCEDURES

Realistic self-consistent calculations on ^{16}O dictate the use of different single-particle energies for the $s_{1/2}$, $p_{3/2}$, and $p_{1/2}$ occupied orbitals. Consequently, ϕ [in Eq. (1.4)] must initially be expressed as a jj coupled ket of two oscillator orbitals:

$$\phi = |n_1 l_1 j_1 n_2 l_2 j_2, JM_J TT_3\rangle. \tag{2.1}$$

These vectors can be transformed into the customary form:

$$\phi = [2(1+\delta_{n_1 l_1 j_1, n_2 l_2 j_2})]^{-1/2} \sum_{jS\mathcal{L}nlN\mathfrak{L}} [1-(-1)^{l+S+T}][(2S+1)(2L+1)(2j_1+1)(2j_2+1)]^{1/2} (-1)^{s+\mathfrak{L}+j+L}[(2j+1)(2L+1)]^{1/2}$$
$$\times \begin{Bmatrix} l & S & j \\ J & \mathfrak{L} & L \end{Bmatrix} \begin{Bmatrix} l_1 & \frac{1}{2} & j_1 \\ l_2 & \frac{1}{2} & j_2 \\ L & S & J \end{Bmatrix} \langle nlN\mathfrak{L}, L | n_1 l_1 n_2 l_2, L\rangle \sum_{m_j m_{\mathfrak{L}}} C^{j\mathfrak{L}J}_{m_j m_{\mathfrak{L}} M_J} | N\mathfrak{L}M_{\mathfrak{L}}\rangle | n(ls)jm_j\rangle | TT_3\rangle, \tag{2.2a}$$

where the $9j$ coefficient transforms the ket from jj to LS coupling; $\langle nlN\mathfrak{L}, L | n_1 l_1 n_2 l_2, L\rangle$ is a Moshinsky-Brody bracket effecting the reduction to relative and center-of-mass coordinates indicated by Eq. (1.12a); and the final $6j$ coefficient recouples S to the relative orbital angular momentum l (as opposed to the total orbital angular momentum L).

The nuclear interaction does not depend on the center-of-mass coordinates, so that $N\mathfrak{L}M_{\mathfrak{L}}$ are good quantum numbers and the $|N\mathfrak{L}M_{\mathfrak{L}}\rangle$ are easily integrated out of all expressions. The component of the wave function for relative coordinates can be written as

$$\langle x | n(lS)jm\rangle = x^{-1} R_{nl}(x) \mathcal{Y}^m_{lsj}, \tag{2.3}$$

where $\mathcal{Y}$ is the (usual) spin-orbit component appropriately vector coupled so that j is a good quantum number. The differential equations that now arise by inserting these components into Eq. (1.4) are of two separate types, each warranting particular attention.

The simpler example is the case of singlet or triplet components with $l=j$. In analogy to Eq. (2.3) we write the correlated wave functions in the form

$$\psi_{n(ls)jm} = x^{-1} u_{nl}(x) \mathcal{Y}^m_{lsj}, \tag{2.4}$$

whereupon Eq. (1.4) reduces to (using the plane-wave propagator)

$$u'' + \left[2\nu(2n+l+\tfrac{3}{2}) - \frac{2\mu}{\hbar^2} W_x - \nu^2 x^2\right] R_{nl} - \left\{[l(l+1)]x^{-2} - \frac{2\mu}{\hbar^2} W_x + \frac{2\mu}{\hbar^2} v_{12}\right\} u = 0, \tag{2.5}$$

where we have set

$$T_{\text{c.m.}} | N\mathfrak{L}\rangle \cong \tfrac{1}{2} E_{N\mathfrak{L}} | N\mathfrak{L}\rangle, \quad \Delta = 0,$$
$$\nu = \mu\omega/\hbar, \quad W_x = (W - \tfrac{1}{2} E_{N\mathfrak{L}}),$$

and μ is the reduced mass of a nucleon.

Triplet states with $j = l \pm 1$ are more complicated, in that they involve the solution of differential equations coupling two components of ψ:

$$\psi_{n(ls)jm} = x^{-1} u_{nl} \mathcal{Y}^m_{lsj} + x^{-1} w_{nl'} \mathcal{Y}^m_{l'sj}, \tag{2.6}$$

where $l' = l+2$ if $j = l+1$ and $l' = l-2$ if $j = l-1$. The resulting coupled differential equations are well known,[8] as are the methods for solution.[3,7,8,14,15] We shall not elaborate on the details here.

Once the correlated wave function ψ has been calculated, Eq. (1.3) can be used to obtain the G matrix elements. Direct integration of

$$\int_0^\infty \phi v \psi d\vec{\mathbf{x}} \tag{2.7}$$

is impractical since at $x \leq c$, ψ is zero while v is infinite. The appropriate limit can be reached with the help of the defect function

$$\chi \equiv \phi - \psi, \tag{2.8}$$

which satisfies the equation

$$(W_x - h_x)\chi = -G\phi = -v\psi, \tag{2.9}$$

where

$$h_x = T_{\text{rel}}.$$

The desired matrix element of G can then be written in the familiar form[3]

$$\langle \phi_\beta | g | \phi_\alpha \rangle = \int_c^\infty \phi_\beta v \psi_\alpha d\vec{\mathbf{x}} + \frac{\hbar^2}{2\mu} \phi^*_\beta(c) \psi^1_\alpha(c) + (\epsilon_\alpha - W_x) \int_0^c \phi^*_\beta \phi_\alpha d\vec{\mathbf{x}} - \nu^2 \frac{\hbar^2}{2\mu} \int_0^c x^2 \phi^*_\beta \phi_\alpha d\vec{\mathbf{x}}. \tag{2.10}$$

A lower case g is used in Eq. (2.10) to emphasize that this is the g matrix in the space of relative coordinates $\vec{\mathbf{x}}_1 - \vec{\mathbf{x}}_2$. To obtain G matrix ele-

ments appropriate to nuclear calculations one must perform two additional operations:
(A) the $Q-1$ corrections, by matrix inversion as indicated in Eq. (1.10);
(B) the transformation from matrix elements in the relative center-of-mass space (to be denoted hereon as RCM) to the properly vector-coupled single-particle space of the two nucleons (to be denoted as SP), as indicated in Eq. (2.2a).
These operations are frequently performed in the order given above, first (A) then (B), as it simplifies the calculations. This procedure is approximate in that it neglects the fact that the Pauli operator Q does not commute with the center-of-mass motion of the two-nucleon system.

Table I compares matrix elements where the $Q-1$ correction was made in the SP space [(B) then (A)], to those performed in RCM space [(A) then (B)]. The difference is seen to be minor in singlet states and in the ^3P states. In the ^3S and ^3D states, however, the difference frequently amounts to nearly an MeV. Consequently, removing the approximation that Q commutes with the center-of-mass motion will make a significant difference in the calculated binding energy of ^{16}O. Therefore, we shall report only calculations done in SP space in the remainder of this paper (in these corrections all states with $2n_i + l_i \leq 6$ are included in the matrix inversion).

It is important to note that since $Q-1$ corrections in the remainder of this paper are all performed in the SP space[16] [(B) then (A)], no definitive physical conclusions may be deduced by examining the relative g matrix elements $\langle n(ls)j|g|n'(l's)j\rangle$. Consequently, in all further discussion (and in the tables) we quote matrix elements either for the two-body jj coupled functions defined by Eqs. (2.1) and (2.2a), or the LS coupled two-body matrix element given by the $9j$ transformation

$$|n_1 l_1 n_2 l_2 LS, JM_J TT_3\rangle = \sum_{j_1 j_2} [(2L+1)(2S+1)(2j_1+1)(2j_2+1)]^{1/2} \begin{Bmatrix} \frac{1}{2} & \frac{1}{2} & S \\ l_1 & l_2 & L \\ j_1 & j_2 & J \end{Bmatrix} \times |n_1 l_1 j_1 n_2 l_2 j_2, JM_J TT_3\rangle. \quad (2.2b)$$

The matrices used to calculate $(Q-1)/(W-H_0)$ are also constructed in the harmonic-oscillator basis, so that the spectrum of particle states is taken as the natural extension of the occupied oscillator orbitals. Thus orthogonality between occupied and unoccupied orbitals is presumed.

Brueckner self-consistency requires that the starting energy W used in the calculation of the reference G matrix element for two states (ik),

$$\langle ik|G_R(W)|ik\rangle, \quad (2.11)$$

be taken as the sum of single-particle energies

$$W = \epsilon_i + \epsilon_k, \quad (2.12)$$

where

$$\epsilon_i = \langle i|T|i\rangle + \sum_{JTk} \tfrac{1}{2}(1+\delta_{ik})(2J+1)(2T+1)(2j_i+1)^{-1} \times \langle ikJT|G(\epsilon_i+\epsilon_k)|ikJT\rangle. \quad (2.13)$$

The net binding energy is then given by

$$\text{B.E.} = \tfrac{1}{2}\sum(\langle i|T|i\rangle + \epsilon_i) - \tfrac{3}{4}\hbar\omega, \quad (2.14)$$

where $\frac{3}{4}\hbar\omega$ represents the kinetic energy of the center of mass. The indices i, k above go over all occupied orbitals.

TABLE I. Comparison of $(Q-1)$-corrected matrix elements $\langle p^2 LSJT|G(W)|p^2 L'SJT\rangle$ (in MeV) in the SP and RCM space. The Hamada-Johnston potential was used; $\hbar\omega = 16.173$ MeV, $W = 3$ MeV. The plane-wave propagator was used in these calculations and in all subsequent tables except for Table VI.

$J\ T\ S\ L\ L'$	SP	RCM
1 0 1 0 0	−8.36	−7.45
1 0 1 0 2	−1.60	−1.57
1 0 1 2 2	−3.86	−3.75
1 0 0 1 1	2.40	2.46
2 0 1 2 2	−7.05	−6.10
3 0 1 2 2	−5.31	−4.68
0 1 0 0 0	−5.59	−5.53
0 1 1 1 1	2.60	2.65
1 1 1 1 1	−0.72	−0.57
2 1 1 1 1	−0.44	−0.30
2 1 0 2 2	−3.89	−3.96

III. PRELIMINARY RESULTS

Before proceeding to the self-consistent calculations a few "numerical experiments" are in order to aid us in the interpretation of results.

TABLE II. Variation of $\langle p^2 LSJT|G(W)|p^2 L'SJT\rangle$ with W. All energies are in MeV. The Hamada-Johnston potential was used, with $\hbar\omega = 12.86$.

$J\ T\ S\ L'\ L \backslash W$	3.00	−17.00	−37.00	−57.00
1 0 1 0 0	−8.22	−7.45	−6.55	−5.73
1 0 1 0 2	−0.87	−1.14	−1.24	−1.28
1 0 1 2 2	−4.00	−3.56	−3.13	−2.75
1 0 0 1 1	1.56	1.59	1.62	1.66
2 0 1 2 2	−6.14	−5.46	−4.90	−4.45
3 0 1 2 2	−4.90	−4.32	−3.81	−3.39
0 1 0 0 0	−5.05	−4.95	−4.74	−4.51
0 1 1 1 1	1.68	1.70	1.72	1.74
1 1 1 1 1	−0.55	−0.51	−0.49	−0.46
2 1 1 1 1	−0.25	−0.21	−0.19	−0.17
2 1 0 2 2	−3.27	−3.17	−3.06	−2.95

First, let us test the sensitivity of the two-body matrix elements to changes in the starting energy (W). This variation is shown in Table II. The interesting feature here is that matrix elements involving the triplet-even interaction (^3S and ^3D states) are found to be most sensitive to W. While W changes from +3 MeV to −57 MeV, for example, the ^3S diagonal matrix element is reduced in magnitude by nearly 2.5 MeV, while the ^1S interaction is altered only by about 0.5 MeV. Likewise, large variations are found in diagonal ^3D matrix elements, while the change in the ^1D and all P-state interactions is hardly significant. The reason for this behavior is most important and not at all difficult to understand.

Variation of the G matrix with the starting energy is given by the wound integral[17]

$$\left\langle \frac{\partial G}{\partial W} \right\rangle = -\int |\phi - \psi|^2 d\vec{\mathbf{x}}. \tag{3.1}$$

This integral is greatest in the relative ($l=0$) triplet S state. This is due to the strong tensor-even interaction. This interaction affects mainly the ^3S and ^3D two-body (LS-coupled) matrix elements. Thus, the sensitivity of the binding energy to the single-particle spectrum can be mainly attributed to the properties of the tensor-even interaction.

It is interesting to make a comparison of the two-body G matrix elements with those obtained by fitting nuclear spectra in shell-model calculations.[18] This is difficult in the self-consistent work, since the $p_{3/2}$ and $p_{1/2}$ hole states have different single-particle energies. Thus, the LS-coupled matrix elements, obtained in shell-model calculation, have different values depending on whether the interacting nucleons are $p_{3/2}^2$, $p_{1/2}^2$, or $p_{3/2}\,p_{1/2}$. Furthermore, it is not at all clear that the self-consistent energy denominator is the appropriate one for comparison with shell-model calculations. Bloch and Horowitz[19] have demonstrated that the effective interaction between valence nucleons in the open-shell nuclei differs from Eq. (1.5) in that the starting energy W should be replaced by E_V:

$$\frac{1}{W-H_0} \to \frac{1}{E_V - H_0}, \tag{3.2}$$

where E_V is the actual energy eigenvalue for the valence particles. Thus, shell-model interactions should have an energy dependence. In practice, it has always been assumed that shell-model calculations are performed over a sufficiently narrow band of energies that an average (constant) energy denominator is appropriate.

This average "starting energy" should lie somewhere between twice the energy of a hole and twice the energy of a particle state (that is, the energy of a p nucleon in ^{5}He). A detailed investigation of this point will be made in a future paper of this series. For the present, we choose $W=3$ MeV as a starting energy for the comparison. This choice derives from the fact that the single-particle energies of the $p_{3/2}$ and $p_{1/2}$ orbitals in ^{5}He are approximately 1 and 4 MeV, respectively. 3 MeV is merely a convenient number of the proper magnitude, and Table II can easily be consulted to check the sensitivity of any particular matrix element to this choice.

Table III shows the G-matrix results with various $\hbar\omega$, compared with matrix elements obtained in shell-model calculations.[20] Only the Hamada-Johnston[21] potential, which gives very nearly the same results as the Yale[22] and Reid[23] hard-core interactions, is shown. Over-all agreement between G-matrix and shell-model results is reasonable and warrants detailed analysis.

Many of the G matrix elements undergo sharp variation with $\hbar\omega$, while many shell-model matrix elements are not well determined by the $1p$ shell data. Nonetheless, excellent agreement is found in the diagonal $^1D_2$, $^1S_0$, $^3P_2$, $^3D_2$, and $^3D_3$, and the off-diagonal $^3S_1$-$^3D_1$ matrix elements. The Hamada-Johnston potential provides a diagonal $^3S_1$ matrix element about 15% short of the shell-model result, which we regard as only fair agreement. Agreement in the $^1P_1$, $^3P_0$, and $^3P_1$ cases is very poor. This might have been anticipated as the most unfavorable case, since the triplet-odd and singlet-odd interactions are not at all well determined by the shell-model calculation. Thus, the excellent agreement found for the $^3P_2$ element

TABLE III. Comparison of $\langle 1p^2SLJT|G|1p^2SL'JT\rangle$ for the Hamada-Johnston potential (MeV) with shell-model results ($W=3$ MeV). Shell-model results are taken from the first paper in this series (Ref. 18). Since several different χ^2 fits to the data were reported, the tabulated value here represents a mean value. Error bars indicate the fluctuation of the matrix elements among these χ^2 fits.

				$\hbar\omega$ (MeV)			
J	T	S	L	L'	11.20	12.86	14.52	Shell-model results
1	0	1	0	0	−7.70	−8.22	−8.62	−9.87±0.20
1	0	1	0	2	−0.70	−0.87	−1.05	−0.80±0.29
1	0	1	2	2	−3.70	−4.00	−4.22	−7.68±0.96
1	0	0	1	1	1.23	1.56	1.92	+8.32±1.19
2	0	1	2	2	−5.45	−6.14	−6.81	−6.15±0.50
3	0	1	2	2	−4.45	−4.90	−5.32	−5.93±0.36
0	1	0	0	0	−4.64	−5.05	−5.38	−5.77±0.23
0	1	1	1	1	1.32	1.68	2.08	0.26±1.64
1	1	1	1	1	−0.46	−0.55	−0.64	+2.35±0.23
2	1	1	1	1	−0.17	−0.25	−0.34	−0.38±0.38
2	1	0	2	2	−2.86	−3.27	−3.67	−2.88±0.52

must be considered, at least in part, to be a stroke of pure fortune. Agreement with the singlet-even and triplet-even components of the interaction, however, is not to be taken so lightly.

More puzzling then, is the rather poor comparison in the diagonal $^3D_1$ matrix element. Although this is the most poorly determined matrix element with even-orbital symmetry in the shell-model fit, it clearly must be at least 2 MeV more attractive than indicated by the G-matrix calculation. The good agreement consistently found with all other components of the triplet-even interaction makes this even more puzzling. It must also be noted that this is the only matrix element where there is a significant difference between the realistic potentials, the Yale potential providing an interaction about 10% more attractive than the Hamada-Johnston potential. The difference appears to be in the balance between the vector spin-orbit and quadratic spin-orbit interactions. The shell-model fit requires a vector spin-orbit even interaction which is very small, and probably opposite in sign to the vector spin-orbit odd interaction. This is closer to the case in the Yale potential.

In all, the comparison between shell-model and G-matrix results is quite favorable. As the shell-model matrix elements are known to yield a very accurate binding energy in ^{16}O (relative to the α-particle core) the prospects for success in the self-consistent calculations appear to be excellent.

IV. RESULTS FOR ^{3}H AND ^{4}He

Self-consistent calculation of ^{3}H by the Brueckner method is most important to the theory of finite nuclei, since the results may be compared with variational calculations of very reasonable accuracy. Since this nucleus does not represent a closed shell, the Goldstone linked-cluster expansion should not be employed, and the Goldstone prescription for the energy denominator is not applicable. Therefore, we use the Bloch-Horowitz[19] energy denominator, which in ^{3}H becomes simply the familiar Brillouin-Wigner prescription[24,25]

$$E = E_0 + \left\langle \phi \middle| v + v\frac{Q}{E - H_0}v + \cdots \middle| \phi \right\rangle. \tag{4.1}$$

Results are shown in Table IV. All of the realistic hard-core interactions yield a binding energy short in magnitude by more than 2 MeV when compared to experiment. The Yale potential yields only a very slightly better value than the Hamada-Johnston potential, while the Reid (hard-core) interaction is short by nearly 3 MeV.

Most important, in Table IV, is the comparison with the variational calculation of Humberston and Hennell.[26] They obtain a binding energy of[27] -6.3 ± 0.5 MeV, in truly remarkable agreement with the value -6.24 MeV obtained in the Brueckner calculation. Thus, it appears that the Brueckner technique is capable of surprisingly accurate results, even in very light nuclei.

In addition to the realistic hard-core interactions, calculations were performed with an effective soft-core potential originally introduced by Goldhammer[25] to investigate second-order perturbation calculations on light nuclei. In ^{3}H the Brueckner calculation yields about $\frac{3}{4}$ of an MeV less binding energy than the perturbation calculation. This seems to be consistent with the high

TABLE IV. Self-consistent results for $A=3$. All energies are in MeV.

Potential	Hamada-Johnston (Ref. 21)	Yale (Ref. 22)	Reid hard core (Ref. 23)	Gold-hammer (Ref. 25)
$\hbar\omega$	12.86	11.20	11.20	16.51
$\langle s^2\,^3S_1 \mid G \mid s^2\,^3S_1\rangle$	−10.74	−10.00	−9.39	−11.70
$\langle s^2\,^1S_0 \mid G \mid s^2\,^1S_0\rangle$	−6.28	−5.39	−5.59	−7.98
Binding energy (this calculation) [a]	−6.24	−6.28	−5.68	−7.75
Binding energy (other calculations)	-6.3 ± 0.5 [b]			−8.48 [c]
Charge radius ^{3}H (in F) (experimental value 1.71 F) [d]	1.55	1.62	1.63	1.54
Ratio charge radii (^{3}He/^{3}H) (experimental value 1.09 ± 0.03) [d]	1.06	1.08	1.07	1.02

[a] Experimental value −8.48 MeV.
[b] See Ref. 26.
[c] See Ref. 25.
[d] See Ref. 29.

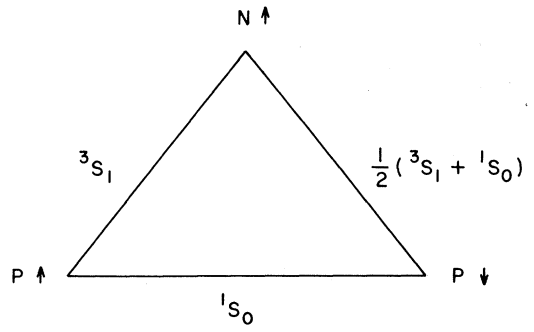

FIG. 1. Schematic diagram of ^{3}He.

degree of accuracy obtained with the Brueckner method for the Hamada-Johnston potential, as second-order perturbation theory will very likely underestimate the repulsive effects of the soft core, thus yielding too much binding.

It is well known that ^{3}H and ^{3}He have different charge radii. In the variational calculations this is normally attributed to the admixture of states with orbital symmetry[28] $[\lambda]=[21]$. The present calculation effects an alternative (although equivalent) description. This description comes about from the fact that the correlated wave functions ψ for the $^3S_1$ and $^1S_0$ two-nucleon states have different radii. The situation in ^{3}He is then shown schematically in Fig. 1, where the distances shown between the nucleons is meant to indicate their rms separation.

The bond between the two protons must be pure $^1S_0$, while the neutron-proton bonds are mixed $^3S_1$-$^1S_0$, as indicated. Thus, this schematic representation is not an equilateral triangle, and the two protons will have an rms distance from the center of mass different from the single neutron. The situation in ^{3}H is obtained by elementary application of the mirror theorem. The derived charge radii are much too small, both in ^{3}H and ^{3}He; however, the ratio is seen to be in fairly reasonable agreement with experiment.[29]

Table V displays the results for ^{4}He. Once again, the hard-core interactions yield too little binding, this time by approximately 11 MeV. Table VI compares binding energies in ^{4}He using the oscillator and plane-wave propagators, along with the Goldstone and Brillouin-Wigner prescriptions for the starting energy. One expects that the plane-wave propagator will yield too much binding (since it allows excited states not orthogonal to ϕ), while the oscillator propagator should yield too little binding (since it neglects $-U$ insertions). The data in Table VI indicate that the binding energy of ^{4}He is not critically sensitive to the energy denominator chosen, and that clearly the Hamada-Johnston potential will not yield nearly enough binding in any case.

V. RESULTS AND ANALYSIS FOR ^{16}O

Table VII shows the results of Brueckner self-consistent calculations on ^{16}O (with the Hamada-Johnston potential) for various values of $\hbar\omega$. Fortunately, the variation of E with $\hbar\omega$ is found to be not at all sharp. E is minimized near $\hbar\omega = 11.20$ MeV, where a 14% alteration in $\hbar\omega$ produces only a 2% variation in E.

We conclude, therefore, that a sensible procedure for determining $\hbar\omega$ is to vary it to minimize the total binding energy. This procedure cannot be taken too seriously, since the method of calculation does not precisely possess the variational property. Nonetheless, if the method represents a good approximation to an exact calculation, the variational property will be at least approximately retained, and should not produce a bad overshoot of the energy eigenvalue. The slow variation of E with $\hbar\omega$ indicates that this is the case. In addition, use of the variational procedure will reveal interesting saturation properties of the hard-core potentials.

The alternative procedure of selecting $\hbar\omega$ to fit the size of ^{16}O appears to be less sensible here. Since it is not certain that the potentials to be tested yield the correct energy, there is no reason to assume *a priori* that they will produce the right size.

TABLE V. Results for ^{4}He using a plane-wave propagator and Goldstone energy denominators. All energies are in MeV. ϵ_s indicates the single-hole self-consistent energy.

Potential	Hamada-Johnston	Yale	Reid (hard core)	Goldhammer
$\hbar\omega$	16.17	16.17	14.51	19.49
$\langle {}^3S_1 \vert G \vert {}^3S_1\rangle$	−10.69	−10.70	−9.48	−13.26
$\langle {}^1S_0 \vert G \vert {}^1S_0\rangle$	−7.22	−7.27	−6.75	−10.03
Binding energy	−17.35	−17.51	−16.06	−26.02
ϵ_s	−14.74	−14.82	−13.47	−20.32

TABLE VI. Results for ^{4}He binding energy with the Hamada-Johnston potential comparing plane-wave and oscillator propagators, along with Goldstone and Brillouin-Wigner energy denominators. All energies are in MeV. Coulomb energies are not included.

	Goldstone denominator	Brillouin-Wigner denominator
Oscillator propagator	−15.34	−17.56
Plane-wave propagator	−17.35	−19.96

TABLE VII. Variation of the binding energy per nucleon (E/A) and single-hole energies (ϵ_j) for ^{16}O as a function of $\hbar\omega$ (Hamada-Johnston potential). All energies are in MeV.

$\hbar\omega$	$-\epsilon(s_{1/2})$	$-\epsilon(p_{3/2})$	$-\epsilon(p_{1/2})$	$-E/A$
7.88	23.89	12.42	11.47	3.46
9.54	27.99	14.33	12.82	3.77
11.20	31.60	15.96	13.75	3.89
12.86	34.69	17.29	14.23	3.81
14.51	37.24	18.31	14.26	3.53
16.17	39.29	19.02	13.87	3.06

Minimized binding energies and self-consistent hole energies are shown in Table VIII, while the corresponding jj coupled matrix elements are given in Table IX. All of the hard-core potentials are seen to fall short of yielding the experimental binding energy, by about 4 MeV/nucleon.[30] As in the case of ^{4}He and ^{3}H the Yale potential yields slightly better results than the Hamada-Johnston potential, at 4.12 MeV/nucleon. Table X clearly demonstrates that there is very little difference between the various modern hard-core interactions.

This result is in very reasonable agreement with previous calculations[7,9,31,32] on ^{16}O with hard-core interactions. It is very disappointing after the good agreement found between the G matrix elements of the Hamada-Johnston potential and the shell-model effective matrix elements (Table III, reviewed in Sec. III), which have been verified to lead to a reasonable binding energy of ^{16}O relative to the α-particle core. To determine where the trouble lies, we now dissect the calculation into its shell-model components.

A first guess as to the source of the trouble is obvious. The G matrix elements in Table III were calculated with $W=3$ MeV, while self-consistent values of W in the $1p$ shell states vary from −32 to −26 MeV. Thus, the larger self-consistent energy denominator will reduce the magnitude of the potential energy. Let us calculate this to see how big the effect is. The potential energy due to the mutual interaction of $1p$ nucleons only is

$$\text{P.E.}(p^{12}) = \sum_{JTj^1} (2J+1)(2T+1) \times \langle p^2 jj^1 JT|\, G\,|p^2 jj^1 JT\rangle . \tag{5.1a}$$

The matrix elements for the Hamada-Johnston potential in Table IX yield

$$\text{P.E.}(p^{12}) = -127 \text{ MeV} . \tag{5.1b}$$

The shell model allows an "experimental" evaluation of this number. The binding energy of ^{16}O relative to the α-particle core (after deducing Coulomb energy) is −113.15 MeV. Shell-model single-particle energies may be taken from the doublet levels of ^{5}He:

$$E(p_{3/2})_{\text{exp}} = 0.96 \text{ MeV} , \tag{5.2a}$$

$$E(p_{1/2})_{\text{exp}} = 3.5 \pm 0.4 \text{ MeV} . \tag{5.2b}$$

It should be noted that the $E(j)$ are not the same as the hole energies $\epsilon(j)$ in the self-consistent calculations. The $E(j)$ represent only the interaction between a $1p$ nucleon and the $1s$ shell core:

$$E(p_j) = \tfrac{5}{4}\hbar\omega + \tfrac{1}{2}(2j+1)^{-1}\sum_{JT}(2J+1)(2T+1) \times \langle s_{1/2}\, p_j JT\,|\, G\,|\, s_{1/2}\, p_j JT\rangle . \tag{5.3}$$

Now one can simply obtain:

$$\text{P.E.}(p^{12})_{\text{exp}} = -113.15 - 2\sum_j (2j+1)E(p_j) , = -134.7 \pm 1.6 \text{ MeV} . \tag{5.4}$$

TABLE VIII. Binding energy and self-consistent single-hole energies in ^{16}O at optimum $\hbar\omega$. All energies are in MeV. No corrections are made for Coulomb effects, and the experimental single-hole energies refer to an odd neutron.

Potential	$\hbar\omega$	$-\epsilon(s_{1/2})$	$-\epsilon(p_{3/2})$	$-\epsilon(p_{1/2})$	$-E/A$
Hamada-Johnston	11.20	31.60	15.96	13.75	3.89
Yale	9.54	28.95	15.18	12.99	4.12
Reid (hard-core)	11.20	30.49	15.53	13.34	3.59
Goldhammer (Ref. 25)	21.15	66.65	32.83	32.19	9.65
Experiment	~16	34 ± 3.5	21.76	15.60	7.98

The agreement between the Hamada-Johnston value for P.E.(p^{12}) and the experimental (shell-model) value is excellent (to within about 5%). Next, let us check the $E(p_j)$ from Eq. (5.3):

$$E(p_{3/2})_{\mathrm{HJ}} \cong 5.4 \text{ MeV}, \tag{5.5a}$$

$$E(p_{1/2})_{\mathrm{HJ}} = 7.0 \text{ MeV}. \tag{5.5b}$$

Comparison of Eqs. (5.2a) and (5.2b) shows very poor agreement, indicating that the Hamanda-Johnston potential does not provide enough attraction between a $1p$ nucleon and the $(1s)^4$ core.

Finally, we compare the $1s$ shell energy:

$$E(s^4) = \tfrac{9}{4}\hbar\omega + \sum_{JT}(2J+1)(2T+1)\langle s^2 JT\,|G|\,s^2 JT\rangle, \tag{5.6}$$

where the center-of-mass kinetic energy $(\frac{3}{4}\hbar\omega)$ has been finally subtracted at this point for appropriate comparison with the α particle. Once again using the matrix elements in Table IX we obtain

$$E(s^4)_{\mathrm{HJ}} \cong -6.5 \text{ MeV}, \tag{5.7}$$

compared with an α-particle binding energy

$$E(s^4)_{\mathrm{exp}} = -28.2 \text{ MeV}. \tag{5.8}$$

The most tenuous point in this analysis is the (shell-model) assumption that the parameters remain constant from nucleus to nucleus. In particular, the "experimental" values of $E(1p_j)$ are open to question, since ^{5}He is unbound. It must be pointed out, however, that shell-model calculations in the $1p$ shell do yield results in very reasonable agreement with a great deal of experimental data, even though the constancy of all parameters is assumed. Such calculations[20, 33, 34] produce single-particle energies in reasonable agreement with the ^{5}He values, and a variation in the parameters sufficiently significant to invalidate the above comparisons is unlikely.

Furthermore, it is illogical to overlook the excellent agreement found between the Hamanda-Johnston and experimental value of P.E.$(1p^{12})$. The detailed comparison between shell model and G matrix elements in Table III strongly contradicts any notion that this agreement is fortuitous.

The calculated binding energy is approximately 64 MeV short of the experimental value. Only about 8 MeV of this shortage is attributable to the interaction between $1p$ nucleons, 22 MeV to the interaction among $1s$ nucleons, and the remaining 34 MeV to interactions between $1s$ and $1p$ orbitals. It is interesting to relate this to average deficiency in the various matrix elements. One has a total of $\frac{1}{2}(16)(15) = 120$ pairs of nucleons, so the calculation is off by about 0.5 MeV/pair. In

TABLE IX. Self-consistent jj matrix elements at optimum $\hbar\omega$ for all the potentials used. Matrix elements and energies are in MeV.

States			Hamada-Johnston	Yale	Reid	Goldhammer
j_1	j_2	$J\ T$	($\hbar\omega = 11.20$)	($\hbar\omega = 9.54$)	($\hbar\omega = 11.20$)	($\hbar\omega = 21.15$)
$0s_{1/2}$	$0s_{1/2}$	1 0	−5.86	−5.31	−5.22	−11.7
		0 1	−4.72	−4.28	−4.86	−10.32
$0s_{1/2}$	$0p_{3/2}$	1 0	−1.26	−1.04	−1.23	−4.03
		2 0	−6.31	−5.63	−5.94	−12.53
		1 1	−2.71	−2.40	−2.76	−6.76
		2 1	−0.59	−0.61	−0.62	0.24
$0s_{1/2}$	$0p_{1/2}$	0 0	−5.99	−5.37	−5.09	−11.85
		1 0	−3.89	−3.43	−3.74	−8.30
		0 1	−1.42	−1.31	−1.76	0.24
		1 1	−0.67	−0.58	−0.65	−3.26
$0p_{3/2}$	$0p_{3/2}$	1 0	−1.52	−1.42	−1.41	−3.61
		3 0	−3.53	−3.21	−3.32	−7.06
		0 1	−2.52	−2.28	−2.54	−5.24
		2 1	−0.98	−0.90	−1.01	−1.93
$0p_{3/2}$	$0p_{1/2}$	1 0	−4.79	−4.35	−4.45	−6.76
		2 0	−4.44	−3.88	−4.37	−10.49
		1 1	−0.41	−0.42	−0.53	0.24
		2 1	−1.85	−1.63	−1.88	−4.11
$0p_{1/2}$	$0p_{1/2}$	1 0	−1.91	−1.84	−1.69	−3.66
		0 1	−0.60	−0.53	−0.57	−0.25
Potential energy			−255.32	−230.42	−250.56	−519.35

the $1p$ shell, there are $\frac{1}{2}(12)(11)=66$ pairs, for a deficit of about 0.1 MeV/pair. Likewise, the $1s$ shell interaction is off by about 3.7 MeV/pair and the $(1s1p)$ matrix elements are short by nearly 0.7 MeV/pair. These numbers are very rough (due to the incorrect kinetic energy), but show a clear trend.

Our interpretation of this trend relates to the relative separation between nucleons. Two $1p$ shell nucleons are, on the average, relatively far apart. Consequently, their interaction is much less sensitive to the short-range part of the potential. The long-range part of the modern hard-core interaction is always taken to be just the one-pion-exchange potential, which must be correct asymptotically. Two $1s$ nucleons are on the average much closer together, hence their interaction is more sensitive to the short-range behavior of the potential. Similarly, a $1s$ and a $1p$ nucleon will have an rms separation intermediate between the $(1s)^2$ and $(1p)^2$, and therefore of intermediate sensitivity to the short-range behavior.

We propose, therefore, that the deficit in the calculated binding energy is due to the short-range part of the hard-core potential. It seems reasonable to conjecture that the hard core is simply too repulsive. This seems plausible, since the exact behavior of the nuclear force at small nucleon-nucleon separations is still clouded in uncertainty. Both soft repulsive cores and momentum-dependent interactions have been frequently proposed as an alternative to the hard core.

To pursue this proposal we examine a soft-core potential calculated by the same method. This soft-core interaction was previously[25] utilized in second-order perturbation theoretic calculation on ^{16}O, yielding a binding of 8.10 MeV/nucleon compared with 9.65 MeV/nucleon obtained here in the Brueckner self-consistent calculation. This potential was employed in a Hartree-Fock calculation by Nesbet,[35] demonstrating that seeking self-consistent single-particle orbitals leads to little improvement over an oscillator variational calculation with this potential. A previous paper[36] reporting opposite conclusions was later found to be in error.[35]

The calculated binding energy of ^{16}O seems to be in very reasonable agreement for this potential, but this is deceptive. To see why, first consider the comparison between G matrix elements for this potential and Hamanda-Johnston at the same starting energy and a value of $\hbar\omega$ appropriate to ^{16}O, which are displayed in Table X. This table shows very little difference between these two sets of matrix elements. Why then does the soft-core porential yield so much more binding energy? As $\hbar\omega$ is increased (decreasing the size), matrix elements of the soft-core interaction increase sufficiently rapidly to compensate for the increase in kinetic energy. The result is that minimum total energy is reached at $\hbar\omega=21.15$ MeV. This yields an rms radius for ^{16}O too small by about 20%. Thus, the potential yields a reasonable binding energy, but at much too high a density. On the other hand, the hard-core potentials saturate at much too small a density. They oversaturate, again indicating that the hard core may be too sharply repulsive.

A more decisive consideration for rejecting the soft-core potential used here is the shell-model dissection. For example, Table IX yields:

$$\text{P.E.}(p^{12})=-248.9\ \text{MeV}, \tag{5.9}$$

a bad overshot which helps to counteract the larger kinetic energy and yields reasonable binding.

Thus, we see that the dissection of the binding energy into its shell-model components provides a powerful tool of analysis. Even if a calculation yields the right binding energy, individual shell-model terms may be poorly reproduced, and the potential used may then be rejected. Clearly, this makes for a much more sensitive test of the potential than simply looking at the binding energy

TABLE X. Comparison of soft core with HJ interaction. $\hbar\omega=14.52$, $W=3$. All energies are in MeV.

$J\ T\ S\ L'\ L$	Hamada-Johnston	Goldhammer
	(p^2)	
1 0 1 0 0	−8.62	−8.51
1 0 0 0 2	−1.05	−0.62
1 0 0 2 2	−4.22	−4.39
1 0 0 1 1	1.92	0.10
2 0 1 2 2	−6.81	−7.67
3 0 1 2 2	−5.32	−5.78
0 1 0 0 0	−5.38	−6.30
0 1 1 1 1	2.08	0.10
1 1 1 1 1	−0.64	0.10
2 1 1 1 1	−0.34	0.10
2 1 0 2 2	−3.67	−4.33
	(sp)	
1 0 0 1 1	1.92	0.10
0 0 1 1 1	−8.48	−8.90
1 0 1 1 1	−9.95	−10.21
2 0 1 1 1	−9.64	−9.96
1 1 0 1 1	−6.23	−6.98
0 1 1 1 1	−1.90	0.1
1 1 1 1 1	2.17	0.1
2 1 1 1 1	−1.05	0.1
	(s^2)	
1 0 1 0 0	−8.83	−8.88
0 1 0 0 0	−6.16	−6.85

and may even be useful in isolating the difficulty within a given interaction.

Because of the importance of the shell-model dissection, we subject it to an additional test. The relation

$$\text{P.E.}(p^{12}) = \sum_j (2j+1)[\epsilon(p_j) - E(p_j)] \tag{5.10}$$

should hold among the experimental shell-model parameters. The $\epsilon(p_j)$ are defined by Eq. (2.13) and should correspond to the separation energies of a $p_{1/2}$ and $p_{3/2}$ neutron from ^{16}O:

$$\epsilon(p_{3/2}) = -21.76 \text{ MeV}, \tag{5.11a}$$

$$\epsilon(p_{1/2}) = -15.60 \text{ MeV}. \tag{5.11b}$$

Insertion of Eqs. (5.11a), (5.11b), (5.2a), and (5.2b) into Eq. (5.10) yields

$$\text{P.E.}(p^{12}) \cong -129.1 \pm 0.8 \text{ MeV}, \tag{5.12}$$

in excellent agreement with the value given in Eq. (5.4). The difference (~5 MeV) is attributable to higher-order G-matrix diagrams, particularly the rearrangement energy.[37]

VI. CONCLUSIONS

The calculations reported in this paper were all performed with Δ [defined in Eq. (1.13)] equal to zero. This choice is highly controversial, since no mathematical prescription for Δ exists in the context of a first-order G-matrix calculation. A definitive determination of Δ must involve rigorous evaluation of three-body diagrams, and this has yet to be carried out in finite nuclei. If this value of Δ is accepted, then one is forced to conclude that the modern hard-core interactions tested do not provide enough attraction to reproduce the experimental binding energy of ^{16}O.

Such a conclusion would be consistent with the following facts:

(a) The binding energy of ^{3}H computed in this paper is in excellent agreement with the variational calculation of Humberston and Hennell, and more than 2 MeV short of the experimental value. The calculation of ^{4}He described above should be of comparable accuracy to the triton, and it is found to be more than 10 MeV short of experiment.

(b) Recent calculations[2,38-41] on nuclear matter indicate that the hard-core interactions yield a binding energy of 8 to 10 MeV per nucleon, while the Reid soft-core potential gives about 11 to 13 MeV. Thus a value of Δ chosen to fit the binding energy of ^{16}O would not be consistent with variational calculations on 1s shell nuclei and results obtained on nuclear-matter calculations by Kallio and Day[42] appear to support the choice $\Delta = 0$.

An additional argument involves the shell-model dissection of ^{16}O presented in Sec. V. This analysis is of such paramount importance that we shall examine its validity once again here. Comparing Eqs. (2.13), (2.14), (5.3), and (5.6) one obtains by straightforward algebra:

$$E(^{16}\text{O}) = E(s^4) + \sum_j (2j+1)[E(p_j) + \epsilon(p_j)]. \tag{6.1a}$$

So far, we have neglected Coulomb corrections. To make a more exacting test of Eq. (6.1a) it is easy to take them into account. It merely entails using different single-particle energies for protons (E^p, ϵ^p) and neutrons (E^n, ϵ^n) so that Eq. (6.1a) becomes

$$E(^{16}\text{O}) = E(s^4) + \tfrac{1}{2}\sum (2j+1)[E^n(p_j) + E^p(p_j) + \epsilon^n(p_j) + \epsilon^p(p_j)]. \tag{6.1b}$$

Substituting the binding energy of the α particle for $E(s^4)$, the single-particle energies of ^{5}He, ^{5}Li for $E^{n,p}(p_j)$, and the separation energies for the p shell protons and neutrons in ^{16}O for $\epsilon^{n,p}(p_j)$ one obtains

$$E(^{16}\text{O}) \cong -122.4 \text{ MeV}. \tag{6.1c}$$

This figure agrees with the experimental value (–127.6 MeV) to an accuracy of 96%.

Comparison should be made between Eq. (6.1a) and Koopmans's equation

$$E(^{16}\text{O}) = \tfrac{1}{2}\sum_i (\langle T_i \rangle + \epsilon_i). \tag{6.2}$$

Equation (6.1a) has two distinct advantages over Eq. (6.2) in nuclei. The first is that all parameters appearing in Eq. (6.1b) are numbers directly obtainable from experiment. In Koopmans's theorem $\langle T_i \rangle$ is not an experimental number; it must be calculated theoretically. The second advantage is that Eq. (6.1a) yields the binding energy of ^{16}O to an accuracy of 96%, while the accuracy is only about 66% with Eq. (6.2).

This improved accuracy is quite a surprise, since Eqs. (6.1a) and (6.2) appear to be derived under identical assumptions. In fact, either equation may be derived from the other by algebraically regrouping terms. This similarity is deceptive, however, because the physical criteria for validity is somewhat different for each equation. In each, one selects a different set of parameters from experiment to calculate $E(^{16}\text{O})$. Let us compare the assumptions carefully.

If Eq. (6.2) holds, then the effective interaction between orbitals must be described by a two-body interaction in all cases. In Eq. (6.1a) it is only essential that the p orbitals are restricted to two-body interactions. In other words if one is forced to go to a higher order in Brueckner theory to cal-

culate the binding so that three-body effective interactions become important then Eq. (6.2) is invalid. Equation (6.1a) would still be valid, however, as long as the important three-body correlations always involved the s shell nucleons. This *may* actually be the case. It is feasible, since s orbitals are crowded closer together in the core compared to the p orbitals in ^{16}O. Thus it seems *a priori* more likely that three s orbitals will strongly interact with each other.

The second criteria for validity in either equation involves whether one can appropriately take parameters from experiment and insert them into the equation. In both cases this procedure is somewhat doubtful. The kinetic energies $\langle T_i \rangle$ are never measured directly, but it is unlikely that an error in the theoretical estimates are serious enough to account for the large discrepancy between Eq. (6.2) and experiment. It may not be legitimate to associate the ϵ_i with the experimental separation energies. This is particularly true for $\epsilon(s)$ where rearrangement energy may be quite important.[37]

Similar objections apply to Eq. (6.1a). In fact the insertion of the various parameters taken from experiment is even more tenuous. For example, $E(s^4)$ is undoubtedly less in magnitude than the binding energy of the α particle. This will be the case since larger starting energies will be used for s orbitals in ^{16}O than in ^{4}He; the Pauli principle excludes additional states into which the s orbitals may scatter when additional nucleons are present, and the size (and shape) of the s orbitals will be altered by the p orbitals yielding a less favorable balance between kinetic energy and s orbital interaction. Similar arguments imply less attractive values for the $E(p_j)$ than experiment would suggest.

These considerations then lead us to believe that substitution of experimental quantities into Eq. (6.1a) should lead to an overestimate of the binding. This is not the case. Equation (6.1c) shows that one in fact comes up with too little binding by about 5 MeV. This discrepancy is very important. It demonstrates that in a calculation on ^{16}O that accounts for only two-body correlations one should never expect to get more binding energy than about 122.4 MeV. The remainder must come from the correlation of three (or more) particles. Thus we have a lower limit on the importance of higher-order correlations in ^{16}O, which appears to be reasonably consistent with the estimate of three-body correlations in nuclear matter[2] (~1 MeV per nucleon). The value for $E(^{16}\mathrm{O})$ will not even be 122.4 MeV, for the reasons listed in the previous paragraph. The question of the validity of Eq. (6.1a) hangs on the magnitude of these effects. In Sec. V we found that for the Hamada-Johnston potential $E(s^4)$ was −6.5 MeV in ^{16}O, compared with a binding energy of −17.35 MeV derived for the free α particle. The alteration in $E(s^4)$ is about 11 MeV. For the soft-core potential of Ref. 23 this alteration is only 6 MeV in going from the α particle to ^{16}O.

Clearly this change in interaction energy is dependent on the potential used. The calculations indicate that the change is too large when the modern hard-core interactions are employed. Perhaps a soft-core potential or a momentum-dependent interaction will yield a more favorable value for $E(s^4)$ in ^{16}O.

Is the agreement between Eq. (6.1b) and experiment fortuitous? It may be; however, it is hard to discount the more detailed agreement between G matrix elements and shell-model results displayed in Table III. Furthermore, an abundance of shell-model calculations are reported in the literature (in the p shell and heavier nuclei) which make the same tacit assumptions that go into Eq. (6.1a). These calculations are known to provide a close description of many detailed nuclear properties such as spectra, ground-state electromagnetic moments, level widths, and spectroscopic factors. A rigorous proof of validity must, of course, await more refined calculations.

If this shell-model analysis is accepted, additional restrictions apply to the parameter Δ, as illustrated by the following example. Becker, Mackellar, and Morris[8] obtain reasonable binding for ^{16}O with the Yale potential setting $\Delta = -66.02$ MeV. Using their matrix elements, one obtains

$$\text{P.E.}(p^{12}) \cong -252 \text{ MeV}, \tag{6.3}$$

which is not in agreement with the value −134.7 ±1.6 MeV obtained in the shell-model analysis [Eq. (5.4)].

Shell-model dissection of the binding energy provides a sensitive test of the interaction. In the calculations presented in Sec. 5, the G matrix elements for two p shell nucleons adequately reproduce P.E.(p^{12}). Thus, if one wants to obtain agreement with all shell-model components of the energy, one would have to introduce different values of Δ in the computation of different G matrix elements. Such a procedure appears far from justifiable; consequently, no alteration of the excited-state spectrum was attempted in this paper.

Higher-order diagrams in the G-matrix expansion must either be calculated or formally demonstrated to be small before any final conclusions can be reached. Core-polarization effects have been calculated in ^{16}O and have been found to be relatively unimportant.[8] A definitive examination has not yet been made for three-body diagrams. The rearrangement energy, in particular, may

prove to be significant.

Finally, we wish to emphasize the importance of checking the binding energy of ^{3}H and ^{4}He with any potential to be tested. If the interaction does not yield reasonable results for the very light nuclei, it seems futile to expect good results in more complex structures. Brueckner theory, as applied here, gave results for ^{3}H in excellent agreement with the more sophisticated variational calculations.[26] It would appear reasonable, therefore, always to check interactions on ^{3}H and ^{4}He by Brueckner theory, since this calculation is relatively very simple.

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