(Invited paper presented at the International Symposium on "Present Status and Novel Developments in the Nuclear Many-Body Problem," Rome, Italy, September 19-23, 1972.)

RECEIVED BY TIC SEP 27 1972

The Renormalized Brueckner-Hartree-Fock Approximation (*)

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Summary. - The renormalization of many-body perturbation theory by factorization of insertions in single-particle (SP) lines having the significance of "true" occupation probabilities is reviewed. The renormalized Brueckner-Hartree-Fock (RBHF) approximation is defined, and its analogue of Koopmans' theorem on the near equality of separation energy centroids and SP energies is demonstrated. The plane wave and harmonic oscillator bases of SP states, and the energy spectrum of the virtual, excited, SP states are discussed. Binding energies, charge densities, and SP energies of light, spherical nuclei obtained with RBHF calculations in the oscillator basis are presented. Corrections to the RBHF approximation, associated with correlations and rearrangement, are considered. Configuration mixing leads to a distribution of SP strength over many eigenstates. Values are given for the second order rearrangement energy, the main contribution to the shift away from the centroid of the eigenstate of greatest SP strength. For deep holes the strength function broadens as $2h-1p$ states, etc. become quasi-degenerate with $1h$ states; as an example, the $(Os)^{-1}$ strength function in ^{16}O is shown. Correlation corrections to the RBHF charge density are discussed. Results of RBHF calculations for nuclei with a neutron excess are cited, and prospects of future improvements in calculations employing the RBHF approximation are contemplated.

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(*) Research sponsored by the U. S. Atomic Energy Commission under contract with Union Carbide Corporation.

1. - Introduction.

The history of quantum electrodynamics has been repeating itself to some extent in recent developments in quantum many-body theory which exhibit a growing appreciation of the power of renormalization. A renormalization of the interaction was accomplished about 18 years ago⁽¹⁾ in response to the evidence that realistic nuclear forces contain rapid radial variations at short distances, and in particular a strong repulsive core. Clearly, perturbation theory in the bare interaction, v , could not converge. The Brueckner reaction matrix, $t(E_S)$, defined by

$$(1.1) \quad t(E_S) = v + v G_0^{\text{out}}(E_S) t(E_S)$$

where $G_0^{\text{out}}(E_S)$ is the unperturbed, two-body propagator $Q^{\text{out}}/[E_S - H^{(0)}]$ in which the Pauli operator, Q^{out} , permits only normally empty states, has proven to be a most useful renormalized (or "effective") interaction. Another major step in the applicability of many-Fermion perturbation theory was the elimination of disconnected diagrams⁽²⁾, which corresponds to the elimination of vacuum fluctuations in quantum field theory. A second renormalization, that of the single-particle (SP) propagators, somewhat analogous to mass renormalization in field theory, has slowly gained recognition. The purpose of this talk is to sketch the nature of one particular propagator-renormalized expansion, that of Brandow, and to show results of some calculations with it. We discuss the lowest order self-consistent field approximation (renormalized Brueckner-Hartree-Fock, RBHF) and the leading correlation corrections to it.

2. - Propagator-unrenormalized, connected-diagram expansions.

2'1. The Goldstone expansion. - Introducing a SP potential, $\mathcal{U}$,

one writes the non-relativistic Hamiltonian for the nucleus as

$$(2.1) \quad \mathcal{K} = \mathcal{K}^{(0)} + \mathcal{K}^{(1)}, \quad \mathcal{K}^{(0)} = \mathcal{T} + \mathcal{U}, \quad \mathcal{K}^{(1)} = \mathcal{V} - \mathcal{U}$$

The unperturbed (independent particle model, IPM) Hamiltonian, $\mathcal{K}^{(0)}$, defines a basis of determinants of SP states, k . In the non-degenerate (closed shell) case, the model ground state, Φ , is the determinant of A SP states, h , of lowest unperturbed energies, $e_h = T_h + U_h$, referred to as normally occupied. Emptying a state h gives a "hole". The SP states unoccupied in Φ are called normally empty or "particle" states. The unperturbed binding energy is

$$(2.2) \quad E^{(0)} = \langle \Phi | \mathcal{K}^{(0)} | \Phi \rangle = \sum_h e_h = \sum_h (T_h + U_h)$$

and the interaction energy is given by the familiar "linked cluster" expansion⁽²⁾

$$(2.3) \quad \Delta E \equiv E - E^{(0)} = \langle \Phi | \mathcal{K}^{(1)} | \Psi \rangle = \sum_{n=0} \langle \Phi | \mathcal{K}^{(1)} \left(\frac{1}{E^{(0)} - \mathcal{K}^{(0)}} \mathcal{K}^{(1)} \right)^n | \Phi \rangle_c,$$

where Ψ is the exact ground state with the intermediate norm $\langle \Phi | \Psi \rangle = 1$, and the subscript c on the matrix element implies that only connected graphs are to be included. Arranged in increasing powers of $\mathcal{K}^{(1)}$, the Feynman-Hugenholtz diagrams (see, e.g. ref. ⁽³⁾) through third order are given in Fig. 1. The SP interaction $-U$ is represented by X , and the antisymmetrized bare two-body interaction, v_A , is represented by the crossing of two lines. A circular line beginning and ending at the same interaction, called a "bubble" is summed only over normally occupied states. We shall define a vertical ordering of "vertices" (interactions); arrows

on lines indicate the direction from creation to destruction; "particle" lines are directed upward, hole lines downward. A Feynman diagram is vertex-unordered: its contribution is the sum of those of the vertex-ordered graphs obtainable from it without altering the topology of the diagram.

The Hartree-Fock (HF) choice of U , namely

$$(2.4) \quad \langle k | U_{\text{HF}} | k' \rangle = \sum_{h_1} \langle k h_1 | v_A | k' h_1 \rangle$$

is equal to the v -interaction with a bubble. It results in the mutual cancellation of all diagrams involving bubbles or X 's except for Fig. 1a and b. Figure 1b is the sum of mutual interaction energies of pairs of uncorrelated nucleons. For any choice of U Fig. 1a cancels the SP potential part of $E^{(0)}$, so the "independent pair model" (I Pair) energy is $E_{\text{IPair}} = \sum_h T_h + \text{Fig. 1b}$, and the remaining "correlation energy" is $E_{\text{corr}} = E - E_{\text{IPair}} = \Delta E - \text{Fig. 1a} - \text{Fig. 1b}$. For the HF choice of U , Fig. 1b is $-\frac{1}{2}$ (Fig. 1a) so E_{IPair} becomes

$$(2.5) \quad E_{\text{HF}} = \sum_h [T_h + \frac{1}{2} U_h].$$

In the HF basis the energy through third order is given in terms of ordinary, vertex-ordered, Hugenholtz diagrams in Fig. 2. The only second order contribution to the HF E_{corr} is Fig. 1d. It is included among the terms of Fig. 2a, which are the leading terms in the expansion of Brueckner reaction matrix elements:

$$(2.6) \quad \text{Fig. 2a} + \dots = \frac{1}{2} \sum_{hh'} \langle hh' | t_A(E_S = e_h + e_{h'}; U_{\text{HF}} | hh' \rangle$$

where U_{HF} is written to remind us that the SP states are in the HF basis.

2'2. The Brueckner-Goldstone expansion in t . - The HF potential is not appropriate for realistic forces. One must define U in terms of t instead of v , and the change of basis will change the values of the t -matrix elements in the generalization of 2.6. For a thorough-going "Bruecknerization" one reorders the Goldstone series so as to sum all "particle-particle" ladders of v -interactions to form t matrices. In the original basic papers^(1,2) Feynman diagrams were not employed and the ladders to be associated with t -matrix elements were not allowed to overlap. For example, the Hugenholtz diagram of Fig. 3a would have associated with it only the diagrams of the form of Fig. 3b. The systematic reordering of the Goldstone series into diagrams of non-overlapping t -matrices yields the Brueckner-Goldstone series. All t -matrices except the highest and lowest are "off the energy shell", meaning that the starting energy, E_s , is not just the sum of the SP energies of the incoming lines but is less than this on-shell value by the virtual excitation energy of the system. Through third order in t and U the Brueckner-Goldstone series for ΔE is given by Fig. 1 with all v 's replaced by t 's and Fig. 1d and the "particle-particle" scattering part of Fig. 1h omitted (they would be redundant; their ladders are already included in those of Fig. 1b).

2'3. The g.t.o. series in t . - Later it was appreciated, apparently first by Thouless⁽⁴⁾, that additional t -matrix elements would be on-shell if some ladders were allowed to overlap. This is a great improvement because on-shell insertions are "factorized", i.e. they can be computed independently of the rest of the diagram. In Fig. 3 suppose one allows

the ladders of the middle t to extend arbitrarily far downward, which includes the possibility of overlapping the ladders of the lowest t . The result is Fig. 3c with all t -matrices on the energy shell. The proof to all orders in v was first derived by Bethe, Brandow, and Petschek⁽⁵⁾ in the time-dependent propagator formalism of Goldstone⁽²⁾. They called the procedure factorization (i.e. placing on the energy shell) by generalized time ordering (g.t.o.). The general rule regarding insertions in SP lines is that they can be factorized by g.t.o. if and only if the external lines of the insertion overlap ("cross")⁽⁶⁾. Thus the t -matrix bubble insertions factorize by g.t.o. for hole-hole scattering, e.g. Fig. 3, and for particle-hole creation or destruction, e.g. the t -matrix analogue of Fig. 1c, e, or f, but not for particle-particle scattering, where only one ordering is possible.

Through third order in t the g.t.o., t -matrix series for ΔE has the same diagrams as the Brueckner-Goldstone series if we reinterpret all intermediate t -matrices with overlapping external lines as being on the energy shell. The mutual cancellation of diagrams analogous to Fig. 1c is achieved with the Brueckner-Hartree-Fock (BHF) potential

$$(2.7) \quad \langle p | U_{\text{BHF}} | h \rangle = \langle h | U_{\text{BHF}} | p \rangle = \sum_h \langle ph_1 | t_A (e_h + e_{h_1}) | hh_1 \rangle.$$

With downward g.t.o. the elimination of the analogue of Fig. 1g is obtained with

$$(2.8) \quad \langle h | U_{\text{BHF}}^\dagger | h' \rangle = \sum_{h_1} \langle hh_1 | t_A (e_h + e_{h_1'}) | h'h_1 \rangle.$$

This can be symmetrized by averaging upward and downward g.t.o. Brandow has shown that this "naive symmetrization" is not adequate, however, for

higher order contributions to $U^{(6)}$.

The choice of "particle - particle" matrix elements of U is of great importance and of considerable controversy. Five approaches come to mind: (i) average off energy shell bubble insertion, i.e. to cancel Fig. 1g (in t) (see, e.g. ref. ⁽⁵⁾); (ii) g.t.o.-factorizable insertions only ⁽⁶⁾, the largest and lowest order one being that of Fig. 7a, which is very small; (iii) compensation of the binding energy of the three-body cluster ⁽⁷⁾; (iv) compensation of the long range v_L -interactions with bubbles plus the energy of the three-body cluster calculated with the t-matrix generated by the short range interaction, v_s ⁽⁸⁾; (v) insertions factorizable by g.t.o. with folds ⁽⁹⁾. Values of the potential energy, $\langle p|U|p \rangle$, used in detailed calculations range from zero (motivated by (ii) or (iii)) to very negative values, e.g. -50 MeV, for low-lying states (motivated by (i), (iv), or (v)). An element of phenomenology is introduced into practical calculations by the necessity to assume values for most of the "particle" spectrum because a self-consistent calculation for all states in any of the approaches described above would be extremely difficult.

2.4. Expectation values of SP operators; the SP density matrix (true occupation probabilities). - Because of the virtual existence of "particles" and holes the normally occupied states are not fully occupied in the exact wave function. The "true" density matrix is defined by

$$(2.9) \quad \rho_{k'k} = \langle \Psi | a_k^\dagger a_{k'} | \Psi \rangle / \langle \Psi | \Psi \rangle.$$

Any SP operator

$$(2.10) \quad \mathcal{O} = \sum_{kk'} \langle k | S | k' \rangle a_k^\dagger a_{k'},$$

has the expectation value

$$(2.11) \quad \langle \mathcal{J} \rangle = \sum_{kk'} \langle k | S | k' \rangle \rho_{k'k} = \text{tr}[\mathcal{J} \rho],$$

so ρ plays a central role. It has a connected-diagram expansion: the sum of all connected diagrams in which $a_k^\dagger a_k$, represented by a dot, occurs once⁽⁴⁾. The terms through third order in this Brueckner-Thouless expansion of $\rho_{k'k}$ are given in terms of Feynman-Hugenholtz diagrams in Fig. 4. Figure 4a gives the IPM (uncorrelated) values

$$\rho_{k'k}^{(0)} = \delta_{kk'} N_k, \quad S^{(0)} = \sum_h \langle h | S | h \rangle$$

where N_k is 1 for $k = h$ and 0 for $k = p$. The two terms of Fig. 4b cancel when BHF self-consistency in the SP wave functions has been achieved. However, in a non-self-consistent reference basis, such as that of a harmonic oscillator or Woods-Saxon potential, Fig. 4b may give the dominant correction to $S^{(0)}$ (see Fig. 9bc). Figure 4c_h gives

$$(2.12) \quad \rho_{h'h}^{(2)} = - \frac{1}{2} \sum_{pp_1 h_1} \frac{\langle h'h_1 | t_A(e_{h'} + e_{h_1}) | pp_1 \rangle \langle pp_1 | t_A(e_h + e_{h_1}) | hh_1 \rangle}{(e_{h'} + e_{h_1} - e_p - e_{p_1})(e_h + e_{h_1} - e_p - e_{p_1})}$$

$$= - \frac{1}{2} \sum_{h_1} \langle h'h_1 | t_A(e_{h'} + e_{h_1}) \frac{Q^{\text{out}}}{e_{h'} + e_{h_1} - \mathcal{K}^{(0)}} \cdot \frac{Q^{\text{out}}}{e_h + e_{h_1} - \mathcal{K}^{(0)}} t_A(e_h + e_{h_1}) | hh_1 \rangle.$$

Further insight into the meaning of $\rho^{(2)}$ may be obtained from two alternative ways of writing (2.12). First, the Bethe-Goldstone correlated two-body state $|\psi_{k_1 k_2}(E_s)\rangle$ is defined by

$$(2.13) \quad v |\psi_{k_1 k_2}(E_s)\rangle = t(E_s) |k_1 k_2\rangle.$$

The wave function $\psi_{k_1 k_2}(E; R, r)$ vanishes rapidly as the separation r decreases within the range of the repulsive core, and this "wound" "heals" as r becomes large. The on-shell "defect" pair state is defined as

$$\begin{aligned}
 (2.14) \quad |\chi_{k_1 k_2}\rangle &= |k_1 k_2\rangle - |\psi_{k_1 k_2}(e_{k_1} + e_{k_2})\rangle \\
 &= \frac{Q^{\text{out}}}{\mathcal{K}^{(0)}(12) - e_{k_1} - e_{k_2}} t(e_{k_1} + e_{k_2}) |k_1 k_2\rangle.
 \end{aligned}$$

Thus,

$$(2.15) \quad \rho_{h'h}^{(2)} = -\frac{1}{2} \sum_{h_1} \langle \chi_{h'h_1}^A | \chi_{hh_1}^A \rangle, \quad \chi_{hh_1}^A \equiv \chi_{hh_1} - \chi_{h_1 h}.$$

A diagonal element corresponds to a depletion, d_h , of a normally occupied state; the second order contribution to the true occupation probability is

$$(2.16) \quad p_h^{(2)} \equiv -d_h^{(2)} \equiv \rho_{hh}^{(2)} = -\frac{1}{2} \sum_{h_1} \langle \chi_{hh_1}^A | \chi_{hh_1}^A \rangle < 0.$$

This depletion, as calculated with realistic nuclear interactions is found to be as large as 10% to 30%.

Secondly, the depletion is related to the energy (frequency) dependence of the effective interaction, t . From (1.1) for $t(E)$ and its adjoint for $t(E')$ we have

$$(2.17) \quad t(E) - t(E') = v \frac{Q^{\text{out}}}{E - \mathcal{H}^{(0)}} t(E) - t(E') \frac{Q^{\text{out}}}{E' - \mathcal{H}^{(0)}} v.$$

If we eliminate the v on the left from the adjoint of (1.1) for $t(E')$ and the v on the right from (1.1) for $t(E)$, we obtain after some cancellation

$$(2.18) \quad \frac{t(E) - t(E')}{E - E'} = - t(E') \frac{Q^{\text{out}}}{(E' - \mathcal{K}(0))(E - \mathcal{K}(0))} t(E).$$

Thus,

$$(2.19) \quad \rho_{h'h}^{(2)} = \sum_{h_1} \frac{\langle h'h_1 | t_A(e_{h'} + e_{h_1}) - t_A(e_h + e_{h_1}) | hh_1 \rangle}{e_{h'} - e_h}.$$

The diagonal elements are

$$(2.20) \quad \begin{aligned} P_h^{(2)} &= - d_h^{(2)} = \frac{\partial}{\partial e_h} \sum_{h_1} \langle hh_1 | t_A(e_h + e_{h_1}) | hh_1 \rangle \\ &= \frac{\partial}{\partial e_h} \langle h | U_{\text{RHF}} | h \rangle < 0. \end{aligned}$$

For the "particle - particle" part of $\rho^{(2)}$, Fig. 4c_p gives

$$(2.21) \quad \begin{aligned} \rho_{p'p}^{(2)} &= \frac{1}{2} \sum_{p_1 h_1 h} \frac{\langle hh_1 | t_A(e_h + e_{h_1}) | pp_1 \rangle \langle p'p_1 | t_A(e_h + e_{h_1}) | hh_1 \rangle}{(e_h + e_{h_1} - e_p - e_{p_1})(e_h + e_{h_1} - e_{p'} - e_{p_1})} \\ &= \frac{1}{2} \sum_{p_1 h_1 h} \langle x_{hh_1}^A | pp_1 \rangle \langle p'p_1 | x_{hh_1}^A \rangle \\ &= \frac{1}{2} \sum_{h_1 h} \langle x_{hh_1}^A | a_p^\dagger(1) a_{p'}(1) | x_{hh_1}^A \rangle \\ &= \frac{1}{4} \sum_{h_1 h} \langle x_{hh_1}^A | a_p^\dagger(1) a_{p'}(1) + a_p^\dagger(2) a_{p'}(2) | x_{hh_1}^A \rangle. \end{aligned}$$

Hence,

$$(2.22) \quad \langle \mathcal{J} \rangle^{(2p)} = \frac{1}{2} \sum_{h_1 h} \langle x_{hh_1}^A | \mathcal{J}(1) \text{ or } \frac{1}{2} [\mathcal{J}(1) + \mathcal{J}(2)] | x_{hh_1}^A \rangle.$$

This lends itself to fairly easy calculation in relative and CM coordinates for operators which separate or factor. The second-order correlation contributions in ${}^4\text{He}$ have been calculated for the rms radius⁽¹⁰⁾, for which $\frac{1}{2}(r_1^2 + r_2^2) = R^2 + \frac{1}{4} r^2$, and for the electron scattering form

factor⁽¹¹⁾, for which $e^{i\vec{q}\cdot\vec{r}_1} = e^{i\vec{q}\cdot\vec{R}} e^{i\vec{q}\cdot\vec{r}/2}$. Calculations of this kind for heavier nuclei are very much needed.

3. - Brandow's propagator-renormalization by g.t.o.-factorization.

Consider the second order in v , g.t.o. insertion of Fig. 5 which consists of the four vertex-ordered contributions, Fig. 5a-5d. If we let $E_1 = e_{h_1} + e_h - e_{p_1} - e_p$ and $E_2 = E_1 + e_{h'} - e_h$, then the denominators in Fig. 5a + 5b are

$$(3.1) \quad \frac{1}{e_h, (e_h, + E_1)} \left[\frac{1}{e_h} + \frac{1}{E_2} \right] = \frac{1}{e_h, e_h} \cdot \frac{1}{E_2}$$

and those of Fig. 5c + 5d are

$$(3.2) \quad \frac{1}{E_1 (e_h, + E_1)} \left[\frac{1}{e_h} + \frac{1}{E_2} \right] = \frac{1}{e_h} \cdot \frac{1}{E_1 E_2}.$$

The contribution of (3.1) is the second order SP self-energy, Fig. 6a. That of (3.2) is quite different; it may be represented as in Fig. 6b, where the hole line, h' , drawn horizontally does not contribute to an energy denominator nor as a hole in the sign rule for diagrams. Because we have performed g.t.o. with extension downward, the insertion, which we recognize as $\rho_{hh'}^{(2)}$, acts at the upper end of the original hole line. The density matrix insertion does not introduce an extra energy denominator into the skeleton, as does a self-energy insertion like Fig. 6a. It simply acts as a weighting factor. An entirely analogous treatment holds for insertions in "particle" lines. Off-diagonal density matrix elements, which vanish by momentum conservation in infinite matter, are expected to be much smaller than diagonal ones. They have been neglected in the calculations performed so far. From now on we shall deal only with the "diagonal ρ approximation".

Brandow's expansion⁽⁶⁾ for the binding energy contains contributions from each irreducible skeleton graph (i.e. each graph of the g.t.o. series which contains no explicit on-shell insertions) with all lines renormalized (i.e. each hole line weighted by P_h and each "particle" line weighted by $1-P_p$, its true emptiness probability). In some cases this results in overcounting the contributions of certain graphs. Claude Bloch has given an elegant topological analysis ("ELC theorem") which solves the overcounting problem for arbitrary choices of propagator renormalization⁽¹²⁾. For Brandow's case the overcounting correction turns out to be minus the true expectation value of the SP, g.t.o.-factorizable self-energy operator⁽⁶⁾. This operator defines the self-consistent SP potential, $U_{g.t.o.}$. Thus the energy is

$$(3.3) \quad E = \sum_h (T_h + U_h) + \mathfrak{A} - \sum_h U_h P_h - \sum_p U_p P_p$$

where $\mathfrak{A}$ is the set of renormalized, irreducible, connected skeleton graphs.

3.1. Stationary properties. - The general form of the energy expression in propagator-renormalized theories immediately implies⁽¹²⁾ certain stationary properties of a kind first discovered in the earliest propagator-renormalized expansion in quantum statistical mechanics⁽¹³⁾. For Brandow's expansion, one regards E as a functional of variable $\tilde{U}_k$'s and $\tilde{P}_k$'s⁽⁶⁾. Then

$$(3.4) \quad \frac{\delta E}{\delta \tilde{P}_k} = \frac{\delta \mathfrak{A}}{\delta \tilde{P}_k} - \tilde{U}_k$$

$$(3.5) \quad \frac{\delta E}{\delta \tilde{U}_k} = \frac{\delta \mathfrak{A}}{\delta \tilde{U}_k} + N_k - \tilde{P}_k.$$

Now differentiation of a graph of $\mathfrak{A}$ with respect to $\tilde{P}_k$ yields an open graph with crossed external lines, k , which therefore contributes to U_k . An example is $\delta/\delta\tilde{P}_h$ applied to renormalized Fig. 1d, which gives Fig. 6a with $h' = h$. Thus, (3.4) vanishes at self-consistency. Next, $\delta\mathfrak{A}/\delta\tilde{U}_k = \delta\mathfrak{A}/\delta\tilde{e}_k$ because $\mathfrak{A}$ depends on $\tilde{U}$ only through the energy denominators. But $\delta/\delta\tilde{e}_k$ applied to a graph of $\mathfrak{A}$ is equivalent to doubling an energy denominator, because

$$\frac{\delta}{\delta\tilde{e}_k} \frac{1}{A\tilde{e}_k} = \frac{\tilde{+} 1}{(A\tilde{e}_k)^2}.$$

This corresponds to inserting a number operator $a_k^\dagger a_k$ at the corresponding level of the graph. The resulting graph is a contribution to P_p or $P_h - N_h$. Thus, at self-consistency (3.5) vanishes. If we write $\mathfrak{A} = \sum_i \mathfrak{A}^{(i)}$, then

$$(3.6) \quad U_k = \sum_i U^{(i)} \text{ with } U^{(i)} = \delta\mathfrak{A}^{(i)}/\delta\tilde{P}_k$$

and

$$(3.7) \quad P_k - N_k = \sum_i P_k^{(i)} \text{ with } P_k^{(i)} = \delta\mathfrak{A}^{(i)}/\delta\tilde{U}_k.$$

Consequently, if one takes a finite truncation of $\mathfrak{A}$, $\mathfrak{A}^T$, and defines U_k^T and P_k^T by (3.6) and (3.7), then E^T has the stationary properties.

3*2. Separation energies. - Let us regard the energy as a functional of the model occupation probabilities, $\tilde{N}_k$, as well as of the $\tilde{U}_k$'s and $\tilde{P}_k$'s (14). The total functional derivative with respect to $\tilde{N}_v$ is

$$(3.8) \quad \frac{d}{d\tilde{N}_v} = \frac{\delta}{\delta N_v} + \sum_k \left[\frac{dU_k}{d\tilde{N}_v} \frac{\delta}{\delta\tilde{U}_k} + \frac{dP_k}{d\tilde{N}_v} \frac{\delta}{\delta\tilde{P}_k} \right].$$

Because of the stationary principles, eqs. (3.4)-(3.7), at self-consistency

$$(3.9) \quad \left(\frac{d}{d\tilde{N}_v} E \right)_{\text{s.c.}} = \left(\frac{\delta}{\delta N} E \right)_{\text{s.c.}} = e_v + \frac{\delta}{\delta N_v} \mathfrak{A}.$$

Equation (3.9) is of the form of the definition of the quasi-particle energy in the Landau theory of Fermi liquids (see, e.g. ref. (3)), which has the significance of a separation energy. However, the first derivative, $\delta E / \delta N_v$, is not the separation energy in a finite system, for which $\Delta N_v = 1$ does not have merely an infinitesimal effect on the system. Instead, if we introduce a superscript [$N_v = 0$ or 1], the eigenseparation (or "adiabatic" separation) energy is

$$(3.10) \quad E_{\text{sep}}(v) = E^{[1]}(v) - E^{[0]}(v) \equiv \frac{\Delta E}{\Delta N_v}.$$

The eigenrearrangement energies $E_{\text{rear}}^{[N_v]}(v)$ are defined by⁽¹⁵⁾

$$(3.11) \quad E_{\text{sep}}(v) \equiv e_v^{[0]} + E_{\text{rear}}^{[0]}(v) = e_v^{[1]} + E_{\text{rear}}^{[1]}$$

so⁽¹⁴⁾

$$(3.12) \quad E_{\text{rear}}^{[0]}(v) = \left(\frac{\delta \mathcal{E}}{\delta \tilde{N}_v} \right)^{[0]} + \frac{1}{2} \left(\frac{d}{d \tilde{N}_v} \frac{\delta E}{\delta \tilde{N}_v} \right)^{[0]} + \dots$$

and

$$E_{\text{rear}}^{[1]}(v) = \left(\frac{\delta \mathcal{E}}{\delta \tilde{N}_v} \right)^{[1]} - \frac{1}{2} \left(\frac{d}{d \tilde{N}_v} \frac{\delta E}{\delta \tilde{N}_v} \right)^{[1]} + \dots$$

Without Taylor expansion

$$(3.13) \quad E_{\text{rear}}^{[1]}(v) = \mathcal{E}^{[1]} - \mathcal{E}^{[0]} - p_v^{[1]} u_v^{[1]} + \sum_{k \neq v} \{ (N_k - p_k^{[1]}) u_k^{[1]} - (N_k - p_k^{[0]}) u_k^{[0]} \}.$$

3.3. Renormalized Brueckner-Hartree-Fock (RBHF) Approximations^(16,17). - An RBHF approximation is obtained from the ordinary BHF approximation by weighting the interacting hole lines by their true occupation probabilities, P_h . The latter may be calculated in various approximations,

the simplest being that of Fig. 4c_h. The strict, g.t.o., RBHF approximation can be derived⁽¹⁴⁾ as a stationary truncation in which $\mathfrak{S}^T$ is given by the two-body cluster

$$(3.14) \quad \mathfrak{S}^{(1)} = \frac{1}{2} \sum_{kk'} N_k N_{k'} \langle kk' | t_A(\{N, U\}; E_s = e_k + e_{k'}) | kk' \rangle P_k P_{k'}.$$

Then from (3.6)

$$(3.15) \quad U_h^{(1)} = \sum_{h'} \langle hh' | t_A(e_{hh'}) | hh' \rangle P_{h'} \equiv U_h^{\text{RBHF}}, \quad U_p^{(1)} \propto N_p = 0$$

and from (3.7)

$$(3.16) \quad P_h - N_h = P_h \sum_{h'} P_{h'} \langle hh' | \left. \frac{\partial t_A(w)}{\partial w} \right|_{w=e_h+e_{h'}} | hh' \rangle$$

and

$$(3.17) \quad P_p = \frac{1}{2} \sum_{hh'} P_h P_{h'} \frac{\partial}{\partial e_p} \langle hh' | t_A(e_h + e_{h'}) | hh' \rangle.$$

It can be shown⁽¹⁴⁾ that (3.17) can be rewritten as

$$(3.18) \quad P_p = \frac{1}{2} \sum_{hh'p'} \frac{|\langle pp' | t_A(e_h + e_{h'}) | hh' \rangle|^2}{(e_h + e_{h'} - e_p - e_{p'})^2} P_h P_{h'},$$

which corresponds to a diagram analogous to Fig. 6b with the dot on a particle line, v's replaced by t's, and the hole lines renormalized.

While the P_p 's are of interest in their own right, in the RBHF approximation they are not needed for the calculation of $\mathcal{U}$, the P_h 's, nor the binding energy. In particular, eq. (3.16) only involves the finite set of hole states and may be solved algebraically. Since

$$(3.19) \quad \mathfrak{S}^{(1)} = \frac{1}{2} \sum_h P_h U_h^{\text{RBHF}}$$

the binding energy (3.5) takes the form

$$(3.20) \quad E_{\text{RBHF}} = \sum_h [T_h + (1 - \frac{1}{2} P_h) U_h],$$

which is very similar to that of the ordinary HF or BHF expression, (2.5), and reduces to it if $P_h \rightarrow 1$.

A generalized RBHF approximation in which "particle"- and hole-line renormalization occur on the same footing has been discussed⁽¹⁴⁾. However, it will be considerably harder to compute with because of the coupling of P_h 's and P_p 's. Because the individual P_p 's are very small ($\lesssim 1\%$) in closed shell nuclei, we think the generalization will be of quantitative interest only for nuclei with a partly open major shell.

3'4. Analogue of Koopmans' theorem for RBHF⁽¹⁵⁾. - Let us consider the "addition energy", eq. (3.10) with v lying outside the core. Because of (3.19) and the fact that $P_h^{[1]} - P_h^{[0]}$ and $T_k^{[1]} - T_k^{[0]}$ are negligible, (3.13) becomes, in the RBHF approximation,

$$(3.21) \quad E_{\text{rear}}^{\text{RBHF}} [1]_{(v_p)} \simeq -\frac{1}{2} P_v U_v^{[1]} + \sum_h (1 - \frac{1}{2} P_h) [U_h^{[1]} - U_h^{[0]}].$$

The potential energy U_h in nucleus $(A+1;v)$ differs from its value in the absence of the valence particle partly in the extra interaction

$$(3.22) \quad X_h = \langle hv | t_A (e_h^{[1]} + e_v^{[1]}) | hv \rangle P_v$$

and partly in slightly different interactions with the other core states,

$$(3.23) \quad C_h = \sum_{h'} P_{h'} \langle hh' | t_A (e_h^{[1]} + e_{h'}^{[1]}) - t_A (e_h^{[0]} + e_{h'}^{[0]}) | hh' \rangle \\ \simeq \sum_{h'} P_{h'} [X_h + C_h + X_{h'} + C_{h'}] \langle hh' | \frac{\partial t_A (e_h + e_{h'})}{\partial e_h} | hh' \rangle.$$

For a nearly static interaction the shift C_h would be negligible, but not so for t in nuclei. An energy derivative of t is related to occupation

probabilities by (3.16), so that

$$(3.24) \quad c_h \simeq (P_h - 1) X_h + P_h \sum_{h'} P_{h'} (X_{h'} + c_{h'}) \langle hh' | \frac{\partial t(e_h + e_{h'})}{\partial e_h} | hh' \rangle$$

in which the first term alone is $\sim 20\%$ of X_h . Summation over h allows another application of (3.16), which gives for the core contribution in

(3.21)

$$(3.25) \quad \sum_h (1 - \frac{1}{2} P_h) c_h \simeq \sum_h (P_h - 1) X_h.$$

Equation (3.21) becomes

$$(3.26) \quad E_{\text{rear}}^{\text{RBHF}} [1]_{(v_p)} \simeq \sum_h \left[-\frac{1}{2} X_h P_h + (1 - \frac{1}{2} P_h) X_h + (P_h - 1) X_h \right] = 0.$$

This is a direct analogue of Koopmans' theorem in HF theory. A similar argument shows the vanishing of the RBHF rearrangement energy for a valence hole. Equation (3.26) is a major improvement over the unrenormalized BHF approximation, for which the rearrangement energies are $\sim 10 \text{ MeV}^{(18)}$. For shell model work and nucleon transfer theory it is very desirable to reduce the rearrangement energies as much as possible⁽¹⁸⁾. Distortions of the core orbitals by the valence particle or hole will contribute an "orbital rearrangement" energy, which has been ignored here.

3.5. Correlation contributions to separation energies; splitting of SP strength⁽¹⁹⁾. - In the RBHF approximation the only renormalized skeleton taken into account is the two-body cluster, eq. (3.14). The higher order diagrams will contribute to binding energies and hence to separation energies. It would be desirable to allow these "correlation" diagrams to influence the self-consistent field, i.e. to work with a higher order, self-consistent truncation. At present this does not appear

computationally feasible. However, one can calculate higher order terms in Δ , in the RBHF basis, as perturbations. The lowest order rearrangement energy is given in Fig. 7a for "particles" and in Fig. 7b for holes. Renormalized hole lines are drawn dashed. Calculations of Fig. 7 for ^{16}O and $^{40}\text{Ca}(19)$ are given in Table I. For the deep hole states the values in parentheses were calculated excluding very close lying intermediate 2h-1p states. The values not in parentheses for the $0s_{1/2}$ holes were calculated carefully, including the close lying virtual 2h-1p states, by treating the energy denominator in a Brillouin-Wigner fashion.

For clarity we should emphasize that the exact $E_{\text{sep}}(v)$ of (3.10) involves an exact eigenstate of the system $A\pm 1$, and is not a centroid or other weighted sum of exact excitation energies. What eigenstate is being referred to? It is the state $\Psi_v^{A\pm 1}$ which will grow out of the state $\Phi_v^{A\pm 1}$ when the residual interaction is turned on. We expect this to be the eigenstate of largest overlap, $\langle \Phi_v | \Psi_v \rangle / \langle \Psi_v | \Psi_v \rangle$, and shall refer to it as the state of greatest or dominant SP strength.

Unfortunately, no information about SP strength is obtained if one limits consideration to the perturbation expansion of the eigenseparation energy, (3.10). Moreover, knowledge of the true occupation probabilities of SP states in the ground state Ψ^A does not provide the SP strengths needed in the theory of transfer reactions; one must know the structure of residual states, $\Psi_v^{A\pm 1}$. Fortunately, a use of the open-shell ("degenerate") formalism, which leads to Brueckner-shell-model calculations, seems to be what is needed. The novelty here is that the cases of interest involve highly excited states, largely uninvestigated heretofore by shell modelists. In the case of a valence hole, one includes along with a 1h configuration, successively more complicated configurations: 2h-1p, 3h-2p, etc. If one considers deeper and deeper 1h states, one encounters

more and more configurations which are quasi-degenerate with it. Each quasi-degeneracy leads to a strong mixing of configurations. One is thereby led to predict an intermediate structure in (p,2p) or (e,e'p) reactions leading to highly excited A-1 nuclei⁽¹⁹⁾. For such a calculation the unperturbed 1h state has an energy relative to the closed shell ground state given by the RBHF single hole energy, $-e_h$. This energy also has the significance of being the centroid of the SP-strength-weighted excitation energies

$$(3.27) \quad -e_h = \sum_n |\langle \phi_{v_h} | \phi_n^{A-1} \rangle|^2 (E_n^{A-1} - E^A),$$

where the ϕ_n 's and E_n 's are the eigenvectors and eigenvalues of the shell model calculation, because the matrix elements of $H^{(1)}$ which mix the configurations are off-diagonal and do not shift the centroid from its unperturbed value⁽¹⁹⁾. Thus, while the exact separation energy, eq. (3.10), is an eigenseparation energy, the RBHF approximation to it is, in the RBHF basis, a centroid energy for the shell model space under consideration. We should note that the RBHF energy, e_h , depends on the size of the model space, because the Q^{out} of the t matrix excludes the "active" SP orbits which are included in the configurations being mixed in the shell model calculation.

Figure 8 shows the $(1/2^+)^{-1}$ spectrum and $(0s_{1/2})^{-1}$ strength distribution between 35 and 60 MeV in ^{15}O as calculated by Becker⁽¹⁹⁾ with the Hamada-Johnston interaction. The shift of the centroid from $-e_{0s_{1/2}}$ is entirely due to the removal of "spurious" states in which the CM is in an excited state; a 0s hole (in the harmonic oscillator basis) is 20% spurious. A strong similarity to the experimental (p,2p) spectrum⁽²⁰⁾,

which has been shifted upward by the Coulomb energy of a Os proton, is seen. It would be very interesting to have high resolution data with which to compare the predicted intermediate structure.

4. - Results of some RBHF calculations in the oscillator basis.

In order to carry out accurate calculations of the reaction matrix, it is almost essential to employ a reference basis of SP states such that pair states can be transformed easily to relative and CM coordinates. The choice is thus between momentum space and the space of harmonic oscillator functions. For light nuclei the oscillator basis has several advantages⁽²¹⁾. The normally occupied and low lying normally empty states may be taken as linear combinations of oscillator states, but the higher lying "particle" states are pure oscillator states. One gives up complete self-consistency regarding these high states, but they are orthogonal to the lower states. A reference spectrum is introduced for the high states. The most widely used has contained the constant shift introduced by Becker and MacKellar (see ref. ⁽²¹⁾), in which $e_p = e_p^{osc} - C$. The well depth C is ~ 50 - 80 MeV. Becker and collaborators have usually determined C self-consistently, for the bottom of the "particle" spectrum, from the average off energy shell bubble (AOESB) insertion. They have also studied the variation of calculated binding energies and SP energies with C . Recent and extensive RBHF calculations by Davies and McCarthy⁽²²⁾ have explored the closed shell nuclei up to ^{208}Pb as a function of C , and of an additional shift, $-B$, for the low lying part of the spectrum. Davies, McCarthy, and collaborators have also written extensively on the techniques of performing matrix-BHF calculations (see the papers cited in ref. ⁽²²⁾).

The results of the RBHF calculations to date seem quite close to

experimental values for light nuclei. For the very light ${}^4\text{He}$ and also for ${}^{12}\text{C}$ and ${}^{16}\text{O}$ it is important to include CM corrections⁽²³⁾. A striking example is the RBHF proton distribution in ${}^4\text{He}$, Fig. 9a⁽²⁴⁾, as calculated from RBHF equations in which the kinetic energy operator includes T_{CM} (method I) or does not include it (method IIC)⁽²³⁾. The preferred method IIC leads to a good rms radius whereas that for method I is too large. The dependence of $\ln|F(q^2)|$, where F is the RBHF electron scattering form factor, on the number of radial $s_{1/2}$ oscillator functions superimposed to give the RBHF 0s state (the "dimensionality", D) is shown for method IIC in Fig. 9b. It is perhaps more informative to plot $F(q^2)$, Fig. 9c, which clearly shows that the theoretical function tends toward the experimental one as D increases, and that $D > 4$ is needed. (The second order correlation correction gives a small positive contribution⁽¹¹⁾.) The form factor provides a severe test of the RBHF orbitals; a D of 3 or 4 is enough to obtain stable values of the binding and SP energies.

Values of the true occupation probabilities are a unique output of RBHF calculations. These, for some "particle" as well as normally occupied states are given in Tables II-IV, along with the energetics, for ${}^4\text{He}$, spherical ${}^{12}\text{C}$, and ${}^{16}\text{O}$. The large (10%) value of P_p for $p = 0p_{1/2}$ in spherical ${}^{12}\text{C}$ suggests that a better unperturbed Φ for the ${}^{12}\text{C}$ ground state would contain configurations with the $0p_{1/2}$ level occupied. This has been accomplished in a generalization of the RBHF approximation to deformed intrinsic states, Φ ⁽²⁵⁾.

Remarks in the earlier sections have warned us that correlation corrections to the RBHF energy functional lead to "rearrangement" contributions to $E_{\text{sep}}^{\text{RBHF}}(v) \approx e_v$, to splitting of SP strength, and to modifications of the charge distribution or electron scattering form factor.

We expect the relative importance of these corrections to increase with the size of the nucleus.

The radius of ^{16}O in Table IV is too small, indicating either that D is too small or that correlation terms relative to RBHF need to be included. The renormalization of the SP potential does decrease the central density and increase the radius (see Fig. 10a for ^{40}Ca , from ref. (22) and Fig. 10b for ^{208}Pb (26)) but not enough for agreement with experiment for $A \geq 16$. Davies and McCarthy have found for ^{16}O , $^{40,48}\text{Ca}$, and ^{208}Pb that as the reference oscillator spectrum is shifted downward, the increase in binding is accompanied by an excessive decrease of radius. They together with Sauer (26) have also tried setting $\langle p|U|p \rangle = 0$ which, for calculations in the oscillator basis leads to $H^{(0)} \rightarrow Q^{\text{out}} T Q^{\text{out}}$ in eq. (1.1). The central density is still much too large (Fig. 10b). Single particle energies also vary with the shift of the excited state spectrum, as shown in Fig. 11, from ref. (22), for the neutron levels just below the Fermi level in ^{208}Pb . The RBHF SP energies should lie lower than the experimental energies given in the first column because the experimental energies refer to eigenstates of ^{207}Pb , and the rearrangement energies are positive (see Table I). A shifted spectrum giving the correct binding energy would lead to SP energies interpolated between columns D and E. Then the rearrangement energy at the Fermi level required to give agreement with experiment would be 3-4 MeV. This is about what would be predicted from Table I. Experimental spin-orbit splittings are not well reproduced by the SP energies. Perhaps the rearrangement energy has a strong j -dependence for holes in spin-unsaturated shells.

The whole purpose of the Brueckner program is to provide, eventually, a correct description of basic nuclear properties without phenomenology

or "fudging". We have seen that at present there are elements of phenomenology in the calculations. Even so, the density distributions for the heavier nuclei are not in very good agreement with experiment, and level separations are not given accurately. Although the renormalization with occupation probabilities has been a considerable step forward, we feel that much is to be gained by further exploration of the full many-body theory, painstaking though it is.

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Figure Captions

Figures 1-7 are explained in the text.

Figure 8. Energy spectrum and single-particle $(0s)^{-1}$ strength of $1/2^+$ states in ^{15}O obtained by mixing $(0s)^{-1}$ and quasi-degenerate $(0p)^{-2} (s-d)^1$ states in a Brueckner-shell-model calculation. From Becker, ref. (19). The two states of the 18-dimensional basis which correspond to an excitation of the CM have been eliminated. The single-particle energies for the s-d shell are those of virtual particles in ^{16}O ; the $0s$ energy is the RBHF energy plus the second order rearrangement energy from far-away configurations. The experimental $(p,2p)$ data for final states in ^{15}N have been shifted by a Coulomb energy for comparison with the calculated spectrum in ^{15}O .

Figure 9a. Proton density in ^4He as calculated from an RBHF Hamiltonian including (I) or not including (II) the kinetic energy of the center of mass. From ref. (24).

Figure 9b. A traditional semilog plot of $|F_{\text{Body}}(q^2)|$ for ^4He vs. q^2 for a pure harmonic oscillator $0s$ state, and for RBHF $0s$ wave functions containing mixtures of 2, 3, or 4 oscillator S-states. CM method II was employed. From ref. (24).

Figure 9c. A replotting of the curves of Fig. 9b; $F_{\text{Body}}(q^2)$ vs. q^2 is given. Experimental values are also given.

Figure 10a. Proton and mass densities for ^{40}Ca calculated with unrenormalized BHF (dashed lines) and RBHF (solid lines). From ref. (22).

Figure 10b. Proton density for ^{208}Pb calculated with unrenormalized BHF (dashed line) and RBHF (dot-dashed line). The RBHF charge density

(convolution of the proton density with the distribution of charge within a proton) is also shown (solid line) for comparison with the experimental charge density (dotted line). From ref. (26).

Figure 11. RBBF energies e_n for the highest occupied neutron levels in ^{208}Pb . From ref. (22). Columns A, B, C, and D are for different choices of level shift of the low lying virtual spectrum, B, and the overall shift $C = 0$. Column E is for $B = 0$ and $C = 7 \text{ MeV}$. A* is for an unnormalized BHF calculation with the same parameters as for A. The values of the binding per nucleon are 8.6(expt.), 2.5(A), 2.7(B), 4.3(C), 5.7(D), and 9.8(E) MeV. The experimental energies are taken from E. Rost: Phys. Letters, 26B, 184 (1968).

Table I. Second Order Rearrangement Energy, Fig. 7, in MeV. From Becker and Patterson, ref. (19).

Single Particle State, $n\ell j$	^{16}O $\alpha=0.45 \text{ F}^{-1}$, $\hbar\omega=16.8 \text{ MeV}$ Hamada-Johnston interaction			^{40}Ca $\alpha=0.356 \text{ F}^{-1}$, $\hbar\omega=10.5 \text{ MeV}$ HF Reid soft core			Nuclear Matter Brueckner-Gammel Thaler interaction k/k_F $s^{(2)}(k)$	
	Unrenorm.	Renorm.		Unrenorm.	Renorm.			
$0s_{1/2}$	(6.2)	(3.4)	13.7		(13.2)	19.5	0.1	27^b
$0p_{3/2}$	2.6	2.1			(4.8)			
$0p_{1/2}$	3.1	2.4			(5.6)		0.9	7^b
$0d_{5/2}$	1.3	1.1			2.1			
$1s_{1/2}$	1.7	1.4			2.0			
$0d_{3/2}$	2.4	1.9			2.1		1.0	4^b
$0f_{7/2}$	0.2	0.2		1.9^a	1.3			
$1p_{3/2}$	0.9	0.7		1.6^a	1.2			
$1p_{1/2}$	0.9	0.7		1.8^a	1.3			
$0f_{5/2}$	0.8	0.6		2.6^a	1.6		1.2	3^b
$0g_{9/2}$					0.3			
$1d_{5/2}$					0.5			
$2s_{1/2}$					0.6			
$1d_{3/2}$					0.5			
$0g_{7/2}$					0.5		2.0	0.6^b

(a) G. F. Bertsch and T. T. S. Kuo: Nucl. Phys., A112, 204 (1968).

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Tables II-IV. RHF results for ${}^4\text{He}$, spherical ${}^{12}\text{C}$, and ${}^{16}\text{O}$. Energies are in MeV, radii and the oscillator range parameter, $b \equiv (\hbar/M\omega)^{1/2}$, in Fermis, and true occupation probabilities in %. The value of the oscillator well depth, C , is that giving self-consistency with the AOESE insertion for low-lying particle states. The SP energies refer to neutron states; "esep" denotes "eigenseparation energy", "cent" denotes "centroid energy", and "res" denotes "resonance energy".

Table II. ${}^4\text{He}$. Reid soft core interaction; $b = 1.088$; $C = 65$; $D = 4$; CM method IIC. From ref. (23).

$$BE/A = -7.08 \text{ (calc)}; -7.05 \text{ (expt)}$$

$$r_{\text{chg}} = 1.62 \text{ (calc)}; 1.63 \pm 0.04 \text{ (expt)}^{(a)}$$

nlj	p_h	e_h	$E_{\text{sep}}^{\text{calc}}(h)^{(b)}$	$E_{\text{sep}}^{\text{exp}}$
$0s_{1/2}$	87	-23.2	-18.9	-20.6 (esep)
		e_v		
$0p_{3/2}$		5.0		~ 1 (res)
$0p_{1/2}$		9.3		~ 5 (res)

(a) H. Frank, et al: Phys. Letters, 19, 391, 719 (errata) (1965).

(b) Includes a CM correction from eq. (6.4) of ref. (23).

Table III. Spherical ^{12}C (not a good model ground state).
 Hamada-Johnston interaction; $b = 1.571$; $C = 45.3$; $D = 3$
 ($l=0$) or 2 ($l=1$); CM method I. From ref. (24). Calc.
 $\text{BE}/A = -5.8$, $r_{\text{chg}} = 2.33$.

<u>$n\ell j$</u>	<u>P_h</u>	<u>e_h</u>
$0s_{1/2}$	78	-39.1
$0p_{3/2}$	80	-13.2 (-16.2 in ^{13}C)
<u>$D = 1$</u>		
	<u>P_p</u>	<u>e_p</u>
$0p_{1/2}$	10.0	-5.3
$1s_{1/2}$	1.2	12.6
$0d_{5/2}$	1.3	14.9
$0d_{3/2}$	1.9	16.3
$1p_{1/2}$	0.6	27.8

2.8 (2.3, $D=3$)
 7.0 (6.4, $D=2$)
 5.8 (6.0, $D=2$)

Table IV. ^{16}O . Hamada-Johnston interaction; $b = 1.571$; $C = 48.6$;
 $D = 3$; CM method IIC. From ref. (23).

$$BE/A = -7.8 \text{ (calc)}, -8.0 \text{ (expt)}$$

$$r_{\text{chg}} = 2.44 \text{ (calc)}, 2.67 \text{ (expt)}$$

nlj	P_h	e_h	$E_{\text{cent}}^{\text{exp}}$	$e_h + E_{\text{rear}}^{(b)}$	$E_{\text{esep}}^{\text{exp}}$
$0s_{1/2}$	78.5	-42.2 (-49) ^(a)	≈ -50	-35	
$0p_{3/2}$	80.5	-22.0		-19.9	-21.9
$0p_{1/2}$	80.0	-18.3		-15.9	-15.7
<div> <div>$D = 1$</div> <div>$D = 3$</div> </div>					
	P_p	e_p	e_v	e_v	$E_{\text{esep}}^{\text{exp}}$
$0d_{5/2}$	1.2	8.7	1.2	-0.98	-4.1
$1s_{1/2}$	1.3	11.0	1.9	-0.77	-3.3
$0d_{3/2}$	2.1	15.7	7.0	3.27	0.9
$0f_{7/2}$	0.1	25.1	16.5		
$1p_{3/2}$	0.6	26.2	15.6		

(a) e_h corrected for CM spuriousity. See Fig. 8.

(b) E_{rear} from Table I.

$$\begin{aligned}
 \Delta F^{[3]} = & \text{(a)} \quad \bigcirc \times + \bigcirc \infty + \left[\text{(b)} \quad \bigcirc \bigcirc + \left[\text{(c)} \quad \bigcirc \times + \bigcirc \times \right] + \text{(d)} \quad \bigcirc \bigcirc \right] \\
 & + \left[\text{(e)} \quad \bigcirc \bigcirc + \triangle + \triangle \times + \triangle \times \right] + \left[\text{(f)} \quad \bigcirc \times + \bigcirc \times + \bigcirc \times \right] \\
 & + \left[\text{(g)} \quad \bigcirc \times + \bigcirc \bigcirc \right] + \text{(h)} \quad \bigcirc \bigcirc + \text{(i)} \quad \bigcirc \bigcirc
 \end{aligned}$$

FIG. 1

$$E^{[3]} = \underbrace{\sum_h T_h + \left[\text{diagram of two circles} \right]}_{\mathcal{E}_{\text{HF}}} + \text{diagram (a)} + \text{diagram (b)} + \text{diagram (c)}$$

(a) (b) (c)

Fig. 2

Fig. 3

Fig. 4

ORNL-DWG 72-9973

Fig. 5

ORNL-DWG 72-9974

(a)

(b)

Fig. 6

Fig. 7

¹⁶O; Mixing of (αα)⁻¹ with Quasi-Degenerate (αp)⁻² (s-d)¹ States. The two Spurious States have been Eliminated. s-d Shell Single Particle Energies are those of Virtual Particles in ¹⁶O; αp 3/2 and αn 3/2 Energies are RBHF (SOC) Energies; and the αα Energy is RBHF (SOC) Plus the 2nd Order Rearrangement Energy from Far-Away Configurations.

Fig. 3

Fig. 2a

Fig. 9b

Fig. 9c

Fig. 10a

Fig. 10b

Fig. 11