One-hole states in double magic nuclei‡

K. Emrich*
Institut für Theoretische Physik der Technischen Universität, Hannover, West Germany

J. G. Zabolitzky†
Institut für Theoretische Physik der Technischen Universität, Hannover, West Germany
and Institut für Theoretische Physik der Ruhruniversität, Bochum, West Germany

K. H. Lührmann
Institut für Theoretische Physik der Ruhruniversität, Bochum, West Germany

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We discuss the equation of motion $\langle\hat{\psi_B}|[H,a_\alpha]|\psi_0\rangle = (\hat{E_B} - E_0)\langle\hat{\psi_B}|a_\alpha|\psi_0\rangle$ in the subspace of states $|\hat{\psi_B}\rangle = \Sigma_\alpha \beta_\alpha a_\alpha|\psi_0\rangle$, where $|\psi_0\rangle$ is the correlated ground state of a double magic nucleus. It is shown that this equation can be solved with high accuracy if some low-order correlation functions of the exp$S$ theory are known. Preliminary results are given for ^{3}H and ^{15}N for four different nucleon-nucleon interactions, i.e., the Reid-soft-core potential with and without the three-body correction of Blatt and McKellar, the Hamada-Johnston potential, and the de Toureill-Sprung supersoft-core potential. The connection with shell model states is discussed.

[NUCLEAR STRUCTURE ^{3}H, ^{15}N, ^{15}O calculated hole states ^{4}He, ^{16}O. Centroid energies from microscopic theory.]

I. INTRODUCTION

Nuclei adjacent to double-magic nuclei show an especially simple structure: There are "dominant" states, the properties of which are (partly) described by the empirical shell model and which are therefore called single-particle shell-model states. These states are usually interpreted to be one-particle or one-hole states of the exact ground state of the double-magic nucleus. In addition to these, there are other types of "one-hole" states, e.g., the Brückner-Hartree-Fock (BHF) and renormalized BHF states.[1,2] The connection between these states and the above mentioned ones is quite complicated because Koopmans's[3] theorem does not hold for nuclei. Dieperink, Brussaard, and Cusson[4] proposed an approach where the connection with experiment is clearer, but unfortunately, it has not yet been applied in calculations going beyond the renormalized BHF. We will show that one can generalize their ansatz in order to obtain an approximation for the dominant states, more strictly speaking, for the energies, form factors, expectation values, and transition probabilities of these states. We will also demonstrate that the exp$S$ theory[5-10] is a very appealing and practical method for solving this problem.

Clearly, one needs a unique definition of a one-hole state. We define a subspace of the $(A-1)$-particle Hilbert space by the states $\{a_\alpha|\psi_0\rangle\}$ (a_α is an annihilation operator) and the one-hole states to be solutions of the Schrödinger equation

$$(H-E_{\hat{B}})|\psi_{\hat{B}}\rangle = 0$$
$$|\psi_{\hat{B}}\rangle = \sum_\alpha \beta_\alpha a_\alpha|\psi_0\rangle \tag{1.1}$$

within this subspace, where $|\psi_0\rangle$ is the exact ground state of the double-magic nucleus and the sum goes over a complete set of single-particle states.

Because it is impossible to solve the full $(A-1)$-particle problem even in this subspace, we solve the equation of motion

$$\langle\psi_{\hat{B}}|[H,a_\alpha]|\psi_0\rangle = (E_{\hat{B}} - E_0)\langle\psi_{\hat{B}}|a_\alpha|\psi_0\rangle \tag{1.2}$$

in the framework of exp$S$ theory. The "sudden-removal" method of Ref. 4 corresponds to a solution of our equation in a one-dimensional subspace.

In Secs. II and III we discuss the connection with "experimental" single-particle wave functions (form factors), etc. We also justify the generalization of the approach of Dieperink *et al.*[4] In Sec. IV we present the method in which (1.2) has been solved and in Sec. V the fragmentation of one-hole states by coupling to excited core states is briefly investigated for ^{15}N. In Sec. VI we present our numerical results. In Sec. VII we discuss the connection with the empirical shell model. Our conclusions will be given in Sec. VIII.

II. FORM FACTORS OF SINGLE-NUCLEON TRANSFER REACTIONS AND SEPARATION ENERGIES

In this section we give some well known definitions of the stripping and pickup form factors, spectroscopic factors, and centroid energies.

The eigenfunctions of an empirical shell-model potential are simple approximations for the form factors[11]

$$\Phi_B(\vec{r}) = (A+1)^{1/2} \int d\xi\, \psi_B(\xi, \vec{r})\psi_0^*(\xi)$$

$$= \sum_\alpha \langle \psi_0 | a_\alpha | \psi_B \rangle \langle \vec{r} | \alpha \rangle , \qquad (2.1a)$$

$$\Phi_B(\vec{r}) = (A)^{1/2} \int \psi_0(\xi, \vec{r})\psi_B^*(\xi) d\xi$$

$$= \sum_\alpha \langle \psi_B | a_\alpha | \psi_0 \rangle \langle \vec{r} | \alpha \rangle \qquad (2.1b)$$

of the deuteron stripping and pickup reactions respectively. $|\psi_0\rangle$ and $|\psi_B\rangle$ are the true states of the A- and $(A \pm 1)$-particle systems (eigenstates of the true Hamiltonian in the complete Hilbert space), ξ stands for the coordinates (and spins) of all nucleons of the residual nucleus, and $\{|\alpha\rangle\}$ is a complete set of one-particle states. In the following we discuss only the form factors of pickup reactions for double-magic nuclei with A nucleons.

Whereas the many-particle states $|\psi_0\rangle$ and $|\psi_B\rangle$ are normalized, the form factors are evidently not. The norm is just the spectroscopic factor

$$S(B) = \langle \Phi_B | \Phi_B \rangle = \sum_\alpha |\langle \psi_B | a_\alpha | \psi_0 \rangle|^2 ; \qquad (2.2)$$

the corresponding energy is the separation energy given by

$$\epsilon_B = E_0(A) - E_B(A-1) . \qquad (2.3)$$

A typical distribution of spectroscopic factors is shown in Fig. 1. Note that in most cases the dominant state is the highest one (which has the lowest excitation energy). The group (a) states, for example, may be interpreted assuming that a one-hole state $\sum_\alpha \gamma_\alpha a_\alpha |\psi_0\rangle$ couples with some core excitation states $|\psi_s\rangle$ in such a way that the one-hole state splits up into states with small spectroscopic factors and a dominant state

$$|\psi_B\rangle = \sum_\alpha \beta_\alpha a_\alpha |\psi_0\rangle + \sum_{s\neq 0} \sum_\alpha \beta_\alpha^s a_\alpha |\psi_s\rangle \qquad (2.4)$$

with small coefficients β_α^s. Therefore, the dominant state $|\psi_B\rangle$ (shell-model state) is often said to be the one-hole state; another approach is to say that the centroid is the one-hole state. Of course both statements are simplifications. It is evident that the true one-hole state defined by (1.1) yields an upper bound on the (negative) energy ϵ_B of the dominant state. On the other hand, if there is a group of states which all have (nearly) the same form factor (up to the normalization constant) and if this group is orthogonal to the form factors of all the states not belonging to it, then the centroid energy

$$\epsilon_{\text{exp}}^{\text{centr.}} = \frac{\sum_B \langle \Phi_B | \Phi_B \rangle \epsilon_B}{\sum_{B'} \langle \Phi_{B'} | \Phi_{B'} \rangle} \qquad (2.5)$$

indeed coincides with the energy $E_0(A) - E_B(A-1)$ given by the solution of Eq. (1.2) in the subspace of one-hole states and the form factor coincides with the wave function calculated from (2.1b) and (1.2). We shall substantiate this remark in Sec. III. A very similar assumption is made in the separation-energy approximation: All the form factors of a "group" are approximated by shell-model functions (more strictly speaking by shell-model functions times spectroscopic factors) which are (up to the asymptotic behavior given by the separation energy) nearly the same for all members of the group. If this approximation holds, the centroid of this group is given by

$$\epsilon_{\text{exp}}^{\text{centr.},\alpha} = \frac{\sum_B S_\alpha(B)\epsilon_B}{\sum_{B'} S_\alpha(B')} , \qquad (2.6)$$

where the "state-dependent spectroscopic factor" $S_\alpha(B)$ is defined by

$$S_\alpha(B) = |\langle \alpha | \Phi_B \rangle|^2 = |\langle \psi_B | a_\alpha | \psi_0 \rangle|^2 . \qquad (2.7)$$

We shall show in the next sections that we can calculate centroids of the form of (2.6) with an arbitrary wave function $|\alpha\rangle$ if we sum over all $(A-1)$-particle states with given j, m, and π.

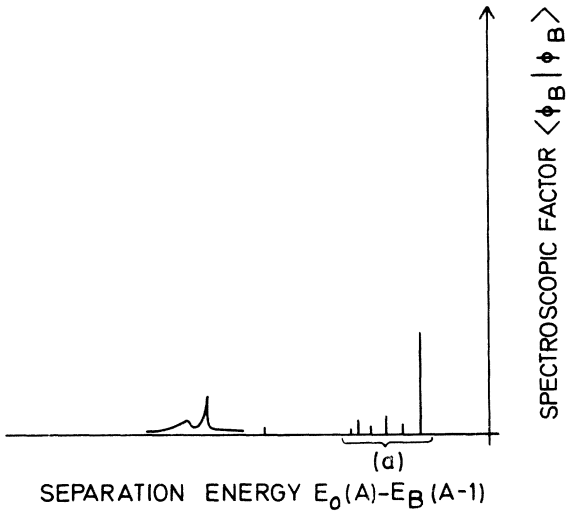


FIG. 1. Schematic distribution of spectroscopic factors of a (double magic -1)-particle nucleus (j, π fixed).

III. ONE-HOLE STATES

In this section we show how the form factors, spectroscopic factors, and centroid energies are associated with the one-hole state. This comparison is continued in Secs. V and VIII.

A direct solution of (1.1) in the subspace of one-hole states, given by

$$|\psi_{\hat{B}}\rangle = \sum_{\alpha'} \beta_{\alpha'} a_{\alpha'} |\psi_0\rangle , \tag{3.1}$$

leads to the equation

$$\sum_{\alpha'} \langle\psi_0| a^\dagger_{\alpha'} H a_\alpha |\psi_0\rangle \beta^*_{\alpha'} = E_{\hat{B}} \sum_{\alpha'} \langle\psi_0| a^\dagger_{\alpha'} a_\alpha |\psi_0\rangle \beta^*_{\alpha'} . \tag{3.2}$$

Unfortunately (3.2) requires the knowledge of two- and three-particle density matrices. One can calculate them, at least in principle, in the frame of expS theory, but the evaluation of the three-particle density matrix would be very difficult. Therefore we subtract from (3.2) the equation

$$\sum_{\alpha'} \langle\psi_0| a^\dagger_{\alpha'} a_\alpha H |\psi_0\rangle \beta^*_{\alpha'} = E_0 \sum_{\alpha'} \langle\psi_0| a^\dagger_{\alpha'} a_\alpha |\psi_0\rangle \beta^*_{\alpha'} \tag{3.3}$$

and obtain

$$\sum_{\alpha'} \langle\psi_0| a^\dagger_{\alpha'} [H, a_\alpha] |\psi_0\rangle \beta^*_{\alpha'} = -\epsilon_{\hat{B}} \sum_{\alpha'} \langle\psi_0| a^\dagger_{\alpha'} a_\alpha |\psi_0\rangle \beta^*_{\alpha'} \tag{3.4}$$

with

$$\epsilon_{\hat{B}} = E_0(A) - E_{\hat{B}}(A-1) . \tag{3.5}$$

Using the definitions

$$D_{\alpha\alpha'} = \langle\psi_0| a^\dagger_{\alpha'} a_\alpha |\psi_0\rangle , \tag{3.6a}$$

$$C_{\alpha\alpha'} = -\langle\psi_0| a^\dagger_{\alpha'} [H, a_\alpha] |\psi_0\rangle , \tag{3.6b}$$

$$|X\rangle = \sum_\alpha \beta^*_\alpha |\alpha\rangle \tag{3.6c}$$

we may write (3.4) as a general eigenvalue problem:

$$(C - \epsilon_{\hat{B}} D)|X\rangle = 0 . \tag{3.7}$$

If the Hamiltonian is given by

$$H = \sum_{\alpha_1\alpha_2} T_{\alpha_1\alpha_2} a^\dagger_{\alpha_1} a_{\alpha_2} + \frac{1}{2} \sum_{\alpha_1\alpha_2\alpha_3\alpha_4} V_{\alpha_1\alpha_2\alpha_3\alpha_4} a^\dagger_{\alpha_1} a^\dagger_{\alpha_2} a_{\alpha_4} a_{\alpha_3} , \tag{3.8}$$

the operator C reads

$$\begin{aligned} C_{\alpha\beta} &= \sum_{\alpha'} T_{\alpha\alpha'} D_{\alpha'\beta} \\ &\quad + \sum_{\alpha_2\alpha_3\alpha_4} V_{\alpha\alpha_2\alpha_3\alpha_4} \langle\psi_0| a^\dagger_\beta a^\dagger_{\alpha_2} a_{\alpha_4} a_{\alpha_3} |\psi_0\rangle \\ &= \langle\alpha| TD |\beta\rangle + \sum_{\alpha'} \langle\alpha\alpha'| VD_2 |\beta\alpha'\rangle , \end{aligned} \tag{3.9}$$

where D_2 is the two-particle density matrix.

Now we would like to discuss the properties of the operators C and D. Using (2.1b) and (2.3) the C operator may be written in the following way:

$$\begin{aligned} C_{\alpha\alpha'} &= \sum\!\!\!\!\!\!\int_{B(A-1)} \langle\psi_0| a^\dagger_{\alpha'} |\psi_B\rangle \langle\psi_B| a_\alpha |\psi_0\rangle \epsilon_B \\ &= \sum\!\!\!\!\!\!\int_{B(A-1)} \langle\alpha|\Phi_B\rangle \langle\Phi_B|\alpha'\rangle \epsilon_B \end{aligned} \tag{3.10}$$

or

$$C = \sum\!\!\!\!\!\!\int_{B(A-1)} |\Phi_B\rangle \langle\Phi_B| \epsilon_B , \tag{3.10a}$$

where the symbol $\sum\!\!\!\!\!\!\int$ means summation over bound states and integration over continuum states and the wave functions $\langle\vec{r}|\Phi_B\rangle$ are given by (2.1b). In close analogy, the one-particle density operator D reads

$$D = \sum\!\!\!\!\!\!\int_{B(A-1)} |\Phi_B\rangle \langle\Phi_B| . \tag{3.11}$$

The operators C and D and the one-hole wave function $\Phi_B(\vec{r})$ are related to the single-particle Green's function. This is shown in the Appendix A. From (3.10) and (3.11) it follows directly that the C and D operators are positive and that the inequality

$$-C \geq D \min_{B(A-1)} |\epsilon_B| \tag{3.12}$$

holds.

The one-hole function corresponding to the $(A-1)$-particle state $|\psi_{\hat{B}}\rangle$ is, of course, not given by the solution $\langle\vec{r}|X\rangle$ of (3.7) but by the function $\Phi_{\hat{B}}(\vec{r})$ resulting from substituting the state $|\psi_{\hat{B}}\rangle$ for the exact eigenstate $|\psi_B\rangle$ in (2.1b):

$$\begin{aligned} \Phi_{\hat{B}}(\vec{r}) &= \sqrt{A} \int d\xi\, \psi_0(\xi, \vec{r}) \psi^*_{\hat{B}}(\xi) \\ &= \sum_\alpha \langle\psi_{\hat{B}}| a_\alpha |\psi_0\rangle \langle\vec{r}|\alpha\rangle \\ &= \sum_{\alpha\alpha'} \langle\psi_0| a^\dagger_{\alpha'} a_\alpha |\psi_0\rangle \beta^*_{\alpha'} \langle\vec{r}|\alpha\rangle . \end{aligned} \tag{3.13a}$$

Employing (3.6c) the corresponding ket is given by

$$|\Phi_{\hat{B}}\rangle = D|X\rangle \tag{3.13b}$$

and the corresponding one-hole strength by[12]

$$S(\hat{B}) = \frac{\langle \Phi_{\hat{B}} | \Phi_{\hat{B}} \rangle}{\langle \psi_{\hat{B}} | \psi_{\hat{B}} \rangle} = \frac{\langle X | D^2 | X \rangle}{\langle X | D | X \rangle} . \tag{3.14}$$

In Appendix B it is shown that (3.7) can be solved in a finite dimensional subspace with any desired accuracy for $|\Phi_{\hat{B}}\rangle$ and $\epsilon_{\hat{B}}$ if the condition

$$S(\hat{B}) \neq 0 \tag{3.15}$$

holds.

States $|\Phi_{\hat{B}}\rangle$ (and $|X\rangle$) belonging to states $|\psi_{\hat{B}}\rangle$ with different symmetry quantum numbers are orthogonal because D and C commute with the operators J^2, J_z, and Π. We stress that different one-particle functions $\Phi_{\hat{B}}(\vec{r})$ belonging to the same quantum numbers j, m, and π are never exactly orthogonal. The orthogonality holds, however, for the $(A-1)$-particle functions $|\psi_{\hat{B}}\rangle$ defined by (3.1) because the metric of (3.7) is given by

$$0 = \langle X_j | D | X_i \rangle = \langle \psi_{\hat{B}_i} | \psi_{\hat{B}_j} \rangle, \quad i \neq j . \tag{3.16}$$

Note that this equation holds also for the case that (3.3) is not strictly valid for a (calculated) state $|\psi_0\rangle$, provided that the operator C is Hermitian.

We return now to the questions of Sec. II. The eigenvalue of (3.7) may be written as

$$\epsilon_{\hat{B}} = \frac{\langle X | C | X \rangle}{\langle X | D | X \rangle} = \frac{\sum_B \langle X | \Phi_B \rangle \langle \Phi_B | X \rangle \epsilon_B}{\sum_{B'} \langle X | \Phi_{B'} \rangle \langle \Phi_{B'} | X \rangle} = \frac{\sum_{B(A-1)} S_x(B) \epsilon_B}{\sum_{B'(A-1)} S_x(B')} . \tag{3.17}$$

One should compare this with (2.6). Once the operators C and D are known, we may also calculate a centroid

$$\epsilon_{\hat{B},\alpha} = \frac{\langle \alpha | C | \alpha \rangle}{\langle \alpha | D | \alpha \rangle} = \frac{\sum_{B(A-1)} S_\alpha(B) \epsilon_B}{\sum_{B'(A-1)} S_\alpha(B')} \tag{3.18}$$

with an arbitrary wave function, e.g., with $|\Phi_{\hat{B}}\rangle$ itself:

$$\epsilon_{\hat{B},\Phi_{\hat{B}}} = \frac{\langle \Phi_{\hat{B}} | C | \Phi_{\hat{B}} \rangle}{\langle \Phi_{\hat{B}} | D | \Phi_{\hat{B}} \rangle} = \frac{\langle X | DCD | X \rangle}{\langle X | D^3 | X \rangle} . \tag{3.19}$$

Other choices are a natural orbital $|n\rangle$ or a Hartree-Fock wave function. For the largest eigenvalue of (3.7) with given j and π the inequality

$$\epsilon_{\hat{B}} \geq \epsilon_{\hat{B},\alpha} \quad \text{with} \quad j_\alpha = j, \ \pi_\alpha = \pi \tag{3.20}$$

is fulfilled for an arbitrary wave function $|\alpha\rangle$, because the expression (3.17) is the maximum of the quotients given by (3.18). Note also that the identity

$$\epsilon_{\hat{B}} = -\frac{\langle \psi_{\hat{B}} | (H - E_0) | \psi_{\hat{B}} \rangle}{\langle \psi_{\hat{B}} | \psi_{\hat{B}} \rangle} \tag{3.21}$$

holds, where the energy E_0 corresponds to the state $|\psi_0\rangle$ which is, in practice, not the exact eigenstate of the Schrödinger equation, but an approximate one.

Of course, for the experimental states with given j and π the inequality

$$\max_{B(j,\pi \text{ given})} \epsilon_B \geq \epsilon_{\hat{B}} \tag{3.22}$$

would hold if the "true" Hamiltonian were used in the calculation of $\epsilon_{\hat{B}}$. Note that the state with the maximum energy is, in general, a "dominant" one (a shell-model state) if states with j, m, and π occur among the occupied states (Fig. 1).

From the very definition of the state $|\psi_{\hat{B}}\rangle$ it is clear that $|\psi_{\hat{B}}\rangle$ is a variational approximation for the states with dominant spectroscopic factors (Fig. 1). This interpretation of $\epsilon_{\hat{B}}$ is, in general, simpler than the interpretation of, e.g., $\epsilon_{\hat{B},\Phi_{\hat{B}}}$ or $\epsilon_{\hat{B},n}$ as a centroid, because experimentalists sum only over part of the states; in order to obtain simple expressions, theorists have to sum over *all* states which are not exactly orthogonal to $|\Phi_{\hat{B}}\rangle$ or $|n\rangle$ (compare, however, Sec. V). If there were a group of states $\{|\psi_{B_a}\rangle\}$ all having the same form factor $\varphi(\vec{r})$ (of course, up to normalization) and if this function $\varphi(\vec{r})$ were orthogonal to the form factors of all other states, then the equations (compare Appendix B)

$$\varphi = \text{const.} |n\rangle = \text{const.} |X\rangle = \text{const.} |\Phi_{\hat{B}}\rangle, \tag{3.23a}$$

$$\epsilon_{\hat{B}} = \epsilon_{\hat{B},n} = \epsilon_{\hat{B},\Phi_{\hat{B}}} = \epsilon_{\text{exp}}^{\text{centr.},n} = \frac{\sum_{B_a} S(B_a) \epsilon_{B_a}}{\sum_{B_a(A-1)} S(B_a)} , \tag{3.23b}$$

$$S(\hat{B}) = \rho_n = \sum_{B_a} \langle \Phi_{B_a} | \Phi_{B_a} \rangle = \sum_{B_a} S(B_a) \tag{3.23c}$$

would hold because $\varphi(\vec{r})$, defined as above, is an eigenfunction of D and C, and therefore also a solution of (3.7).

The fact that $|\psi_{\hat{B}}\rangle$ is a variational approximation of the exact state $|\psi_B\rangle$ is the main reason why we generalized the work of Dieperink *et al.*[4] Another reason is that we hope to obtain wave functions $\Phi_{\hat{B}}(\vec{r})$ which resemble the empirical form factors of the dominant states more closely than the natural orbitals do.

We end this section with a rather trivial remark about the asymptotic behavior of $\Phi_{\hat{B}}(\vec{r})$. From (3.7), (3.9), and (3.13) it follows that for neutrons the radial part of the form factor $\Phi_{\hat{B}}(\vec{r})$ asymptotically goes over into the Hankel function $h^{(1)}[i(2\mu|\epsilon_{\hat{B}}|)^{1/2} r]$; for proton-hole nuclei the asymptotic form is given by the corresponding Coulomb function if the two-particle density matrix is replaced by the antisymmetrized product of one-particle density matrices; this should be a good approximation in the asymptotic region.

IV. EVALUATION OF THE ONE-PARTICLE DENSITY MATRIX AND OF THE C MATRIX IN THE exp$S$ FORMALISM

In this section we present the method by which we calculated the density matrices and the matrix C defined by (3.6b). Our computation of the one-particle density and of the C matrix (3.9) is based on the knowledge of the ground-state vectors $|\psi_0\rangle$ of ^{4}He, ^{16}O, and ^{40}Ca. The necessary information about these state vectors has been computed using the exp$S$ formalism.[5-10] Since an extensive review of the formalism and of these calculations has been given,[10] we will give here only a brief comment. The formalism is based on representation of the state vector by

$$|\psi\rangle = \exp(S)|\Phi\rangle \quad \left(\frac{|\psi\rangle}{\langle\psi|\psi\rangle^{1/2}} = |\psi_0\rangle\right), \tag{4.1a}$$

where Φ is a Slater determinant and S is the sum of particle-hole excitation amplitudes

$$S = \sum_{n=1}^{A} S_n ,$$

$$S_n = \frac{1}{(n!)^2} \sum_{\nu_i \rho_i} \langle \rho_1 \cdots \rho_n | S_n | \nu_1 \cdots \nu_n \rangle_A \times a^\dagger_{\rho_1} \cdots a^\dagger_{\rho_n} a_{\nu_n} \cdots a_{\nu_1} . \tag{4.1b}$$

Here $\nu, \mu, \lambda(\rho,\sigma,\tau)$ label normally occupied (unoccupied) states and the labels α, β, γ are used for both kinds of states. A is the number of particles. As a subscript A means antisymmetrization without normalization, e.g.,

$$|\nu_1\nu_2\rangle_A = |\nu_1\nu_2\rangle - |\nu_2\nu_1\rangle .$$

The exp$S$ hierarchy constitutes a set of nonlinear coupled equations for the amplitudes $\langle S_n\rangle$ which is equivalent to the Schrödinger equation. In the following the results of two truncations [GBHF and FBHF(3)] of these equations will be used. Assuming that the reader is familiar with Brueckner theory we remark that GBHF (generalized Brueckner-Hartree-Fock) calculations are closely related to Brueckner-Hartree-Fock calculations (the effects of hole-hole scattering and some other diagram classes are included in addition). In FBHF(3) (Faddeev-Brueckner-Hartree-Fock) the three-body Bethe-Faddeev equation is incorporated *self-consistently*. In terms of Goldstone diagrams this introduces the particle potential to all orders into the two-body equation and sums many other diagram classes. The amplitude $\langle S_2\rangle$ would be the usual defect function in the truncation where we only have the Brueckner-Hartree-Fock (BHF) equations and thus our parameter

$$\langle \nu | \kappa | \nu \rangle = \sum_{\mu} \langle \nu\mu | S_2^\dagger S_2 | \nu\mu \rangle_A \tag{4.2}$$

is a generalization of the usual "convergence" parameter[1] κ. In FBHF(3) calculations it is up to 40% larger than in BHF calculations (depending on the NN potential). Still it is argued[10] that convergence seems to be very good and that taking into account higher-order equations should not change the results appreciably.

In the exp$S$ equations the so called "reduced subsystem amplitudes" $\langle \chi_n^{ij}\rangle$[10,13] are of some interest. They are the simplest quantities in terms of $\langle S\rangle$ amplitudes where $\langle V_{ij}\chi_n^{ij}\rangle$ remains always finite in the case of a hard core potential. Wherever V_{ij} occurs in the exp$S$ equations it occurs as $\langle V_{ij}\chi_n^{ij}\rangle$. $\langle\chi_2\rangle$ is a "generalized" Bethe-Goldstone wave function and $\langle\chi_3\rangle$ is related to the Bethe-Faddeev amplitude. In terms of $\langle S\rangle$ amplitudes the $\langle\chi_n^{ij}\rangle$ are given by

$$\langle \alpha_1\alpha_2\sigma_3\cdots\sigma_n | \chi_n^{(12)} | \nu_1\cdots\nu_n\rangle_A = \langle \Phi | a^\dagger_{\nu_1}\cdots a^\dagger_{\nu_n} a_{\sigma_n}\cdots a_{\sigma_3} e^{-S} a_{\alpha_2} a_{\alpha_1} e^S | \Phi\rangle , \tag{4.3a}$$

$$\langle \alpha_1\alpha_2 | \chi_2 | \nu_1\nu_2\rangle_A = \langle \alpha_1\alpha_2 | \nu_1\nu_2\rangle_A + \langle \alpha_1\alpha_2 | S_2 | \nu_1\nu_2\rangle_A , \tag{4.3b}$$

$$\langle \alpha_1\alpha_2\rho_3 | \chi_3^{(12)} | \nu_1\nu_2\nu_3\rangle_A = A_\nu(\langle\alpha_1\rho_3|S_2|\nu_1\nu_3\rangle\langle\alpha_2|\nu_2\rangle) + A_\nu(\langle\alpha_2\rho_3|S_2|\nu_2\nu_3\rangle\langle\alpha_1|\nu_1\rangle) + \langle\alpha_1\alpha_2\rho_3|S_3|\nu_1\nu_2\nu_3\rangle_A . \tag{4.3c}$$

Here A_ν antisymmetrizes with respect to the labels ν, e.g.,

$$A_\nu(|\nu_1\nu_2\rangle|\nu_3\rangle) = |\nu_1\nu_2\rangle_A|\nu_3\rangle - |\nu_1\nu_3\rangle_A|\nu_2\rangle - |\nu_3\nu_2\rangle_A|\nu_1\rangle .$$

It should be noted that the $\langle S_n\rangle$ are zero if on the left (right) hand side there is a normally occupied (unoccupied) state label. In writing (4.3) we have assumed

$$\langle S_1\rangle \equiv 0 \Longleftrightarrow \langle\Phi|\psi\rangle = \max , \tag{4.4}$$

which is the maximum overlap condition.[6,10] (4.4) is a condition for the Slater determinant Φ and implies that the single-particle particle states have to be determined self-consistently. In the formalism developed here and in our calculations this condition is always used. It makes the expansion of the density matrix simpler.

Computation of a "true quantity" like the density $\langle D_n\rangle$ is much more delicate than computation of a model quantity like $\langle\chi_n\rangle$. This is clearly seen if we look at the energy which in the exp$S$ formalism is computed as "model energy":

$$E_{\text{model}} = \langle\Phi|T|\psi\rangle + \langle\Phi|V|\psi\rangle$$

$$= \sum_{\nu} \langle\nu|T|\nu\rangle + \frac{1}{2}\sum_{\nu\nu'}\langle\nu\nu'|V\chi_2|\nu\nu'\rangle_A . \qquad (4.5a)$$

The "true" energy

$$E_{\text{true}} = \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle}$$

$$= \sum_{\alpha\beta} \langle\beta|T|\alpha\rangle\langle\alpha|D_1|\beta\rangle$$

$$+ \frac{1}{2}\sum_{\beta_i\alpha_i}\langle\beta_1\beta_2|V|\alpha_1\alpha_2\rangle\langle\alpha_1\alpha_2|D_2|\beta_1\beta_2\rangle , \qquad (4.5b)$$

$$\langle\alpha_1\cdots\alpha_n|D_n|\beta_1\cdots\beta_n\rangle = \frac{\langle\psi|a^\dagger_{\beta_1}\cdots a^\dagger_{\beta_n}a_{\alpha_2}\cdots a_{\alpha_1}|\psi\rangle}{\langle\psi|\psi\rangle} ,$$

$$D_1 = D$$

should have the same value, but the expectation values of the kinetic and potential energies have much larger absolute values than the corresponding model quantities. In our C matrix (3.9) both D_1 and D_2 are needed and we regard it as quite important to take this cancellation into account.

The conditions for our density matrix are[14]

(i) $E_{\text{true}} = E_{\text{model}}$,

(ii) $$\sum_{\alpha_1\alpha_2}\langle\alpha_1\alpha_2|D_2|\alpha_1\alpha_2\rangle$$

$$= (A-1)\sum_{\alpha_1}\langle\alpha_1|D_1|\alpha_1\rangle$$

$$= (A-1)A \quad \text{[trace conversation (Ref. 15)]} ,$$

(iii) $D_n^\dagger = D_n$ (Hermiticity).

In Ref. 14 it is shown that conditions (i) and (ii) are fulfilled explicitly in the expansion of the density matrix we will now give. For condition (i) this is shown by relating the truncation of the equations [here FBHF(3)] to a truncation of the density matrix. The same truncations are used for varying the true energy (4.5b) to obtain the truncated equations and for the density matrix given here. According to Ref. 14 condition (i) is fulfilled if we put

$$\langle\rho_1\cdots\rho_n|D_n|\nu_1\cdots\nu_n\rangle = 0 \quad \text{for } n \geq 3$$

and (4.6)

$$\langle S_n\rangle = \langle\chi_n\rangle = 0 \quad \text{for } n \geq 4 ,$$

which we will use in the following. We remark that, in general, condition (iii) is only fulfilled explicitly for the nondiagonal elements

$$\langle\rho_1\cdots\rho_n|D_n|\nu_1\cdots\nu_n\rangle$$

of the density matrix. We use (4.6) in writing the expansion but it will not become more complex by including higher-order terms.[14] To obtain the expansion for the one-body density matrix we use, in a first step,

$$1 = e^S e^{-S}$$

and write

$$\langle\alpha|D_1|\beta\rangle = \frac{\langle\Phi|e^{S\dagger}e^S e^{-S}a^\dagger_\beta a_\alpha e^S|\Phi\rangle}{\langle\Phi|e^{S\dagger}e^S|\Phi\rangle} . \qquad (4.7)$$

Then we insert a unit operator

$$1 = |\Phi\rangle\langle\Phi| + \sum_{n=1}^{A}\frac{1}{(n!)^2}a^\dagger_{\rho_1}\cdots a^\dagger_{\rho_n}a_{\nu_n}\cdots a_{\nu_1}|\Phi\rangle$$

$$\langle\Phi|a^\dagger_{\nu_1}\cdots a^\dagger_{\nu_n}a_{\rho_n}\cdots a_{\rho_1} \qquad (4.7a)$$

to obtain the expansion

$$\langle\alpha|D_1|\beta\rangle = \langle\Phi|e^{-S}a^\dagger_\beta a_\alpha e^S|\Phi\rangle + \sum_{n\rho_i\nu_i}\frac{1}{(n!)^2}\langle\nu_1\cdots\nu_n|D_n|\rho_1\cdots\rho_n\rangle\langle\Phi|a^\dagger_{\nu_1}\cdots a^\dagger_{\nu_n}a_{\rho_n}\cdots a_{\rho_1}e^{-S}a^\dagger_\beta a_\alpha e^S|\Phi\rangle . \qquad (4.8)$$

Using

$$e^{-S}Oe^S = O + [O,S] + \frac{1}{2!}[[O,S],S] + \cdots \qquad (4.9)$$

this is easily evaluated and we get

$$\langle\nu|D_1|\mu\rangle = \langle\nu|\mu\rangle - \sum_{\nu_1\sigma_1\sigma_2}\langle\nu\nu_1|D_2|\sigma_1\sigma_2\rangle\langle\sigma_1\sigma_2|S_2|\mu\nu_1\rangle - \cdots , \qquad (4.10a)$$

$$\langle\rho|D_1|\tau\rangle = \sum_{\nu_1\nu_2\sigma_1}\langle\nu_1\nu_2|D_2|\tau\sigma_1\rangle\langle\rho\sigma_1|S_2|\nu_1\nu_2\rangle + \cdots . \qquad (4.10b)$$

A diagrammatic representation of (4.10) is given in Fig. 2.

For $\langle\rho|D_1|\nu\rangle$ we use a different expansion which is developed by writing

$$\langle\rho|D_1|\nu\rangle = \frac{\langle\Phi|e^{S\dagger}a^\dagger_\nu e^S e^{-S}a_\rho e^S|\Phi\rangle}{\langle\Phi|e^{S\dagger}e^S|\Phi\rangle} \qquad (4.11)$$

and inserting a unit operator in $(A-1)$-particle space

$$1_{A-1}=\sum_{\mu} a_{\mu}|\Phi\rangle\langle\Phi|a_{\mu}^{\dagger}+\sum_{\substack{n=1\\ \mu\rho_i\nu_i}}^{A-1}\frac{1}{n!(n+1)!}a_{\rho_1}^{\dagger}\cdots a_{\rho_n}^{\dagger}a_{\nu_n}\cdots a_{\nu_1}a_{\mu}|\Phi\rangle\langle\Phi|a_{\mu}^{\dagger}a_{\nu_1}^{\dagger}\cdots a_{\nu_n}^{\dagger}a_{\rho_n}\cdots a_{\rho_1}. \tag{4.12}$$

We get

$$\langle\rho|D_1|\nu\rangle=\sum_{\mu\nu_1\rho_1}\langle\mu\nu_1|D_2|\nu\rho_1\rangle\langle\rho\rho_1|S_2|\mu\nu_1\rangle+\frac{1}{2}\sum_{\mu\nu_i\rho_i}\langle\mu\nu_1\nu_2|D_3|\nu\rho_1\rho_2\rangle\langle\rho\rho_1\rho_2|S_3|\mu\nu_1\nu_2\rangle+\cdots. \tag{4.13}$$

$\langle\nu|D_1|\rho\rangle$ is then determined by condition (iii). (4.13) is represented by diagrams in Fig. 3.

Equations (4.10) and (4.13) are determined mainly by the two-body density matrix which we will now evaluate. The basic expansion is obtained by writing

$$\langle\alpha_1\alpha_2|D_2|\beta_1\beta_2\rangle=\frac{\langle\Phi|e^{S^+}a_{\beta_1}^{\dagger}a_{\beta_2}^{\dagger}e^{S}e^{-S}a_{\alpha_2}a_{\alpha_1}e^{S}|\Phi\rangle}{\langle\Phi|e^{S^+}e^{S}|\Phi\rangle}. \tag{4.14}$$

Inserting a unit operator in $(A-2)$-particle space [similar to (4.12)] and using the definition of the $\langle\chi_n\rangle$ we get

$$\langle\alpha_1\alpha_2|D_2|\beta_1\beta_2\rangle=\sum_{\mu_1\mu_2}\langle\mu_1\mu_2|D_2|\beta_1\beta_2\rangle\langle\alpha_1\alpha_2|\chi_2|\mu_1\mu_2\rangle+\frac{1}{2}\sum_{\mu_i\rho_3}\langle\mu_1\mu_2\mu_3|D_3|\beta_1\beta_2\rho_3\rangle\langle\alpha_1\alpha_2\rho_3|\chi_3^{(12)}|\mu_1\mu_2\mu_3\rangle+\cdots. \tag{4.15}$$

$\langle\alpha_1\alpha_2|D_2|\nu_1\nu_2\rangle$ and [by condition (iii)] also $\langle\nu_1\nu_2|D_2|\alpha_1\alpha_2\rangle$ are determined from (4.15). They are given diagrammatically in Fig. 4. It is worthwhile to look closer at Fig. 4. $\langle\alpha_1\alpha_2|D_2|\nu_1\nu_2\rangle$ may be regarded as the true quantity corresponding to the model quantity $\langle\alpha_1\alpha_2|\chi_2|\nu_1\nu_2\rangle_A$. The first term in the expansion of $\langle D_2\rangle$ is seen to be $\langle\chi_2\rangle$ weighted with the probability that the hole lines entering $\langle\chi_2\rangle$ are occupied. In second and other higher-order terms $\langle\chi_3\rangle, \langle\chi_4\rangle, \ldots$ are introduced. They are also weighted with quantities which measure the probability with which the hole states and particle-hole excitations really occur. These are just standard constituent features of the difference between model and true quantities.

To get a solvable system of equations for the density matrix we still need expansions for $\langle\mu\nu_1|D_2|\nu\rho_1\rangle$, $\langle\mu\nu_1\nu_2|D_3|\nu\rho_1\rho_2\rangle$, $\langle\mu_1\mu_2|D_2|\nu_1\nu_2\rangle$, and $\langle\mu_1\mu_2\mu_3|D_3|\nu_1\nu_2\rho_3\rangle$. These expansions can be obtained in different ways; if we want to fulfill conditions (i) and (ii) we have to expand as in (4.7), inserting the unit operator in A-particle space (4.7a). We get

$$\langle\mu\nu_1|D_2|\nu\rho_1\rangle=A_{\mu\nu_1}(\langle\mu|\nu\rangle\langle\nu_1|D_1|\rho_1\rangle)+\cdots, \tag{4.16a}$$

$$\langle\mu\nu_1\nu_2|D_3|\nu\rho_1\rho_2\rangle=A_{\mu\nu_i}(\langle\mu|\nu\rangle\langle\nu_1\nu_2|D_2|\rho_1\rho_2\rangle)+\cdots, \tag{4.16b}$$

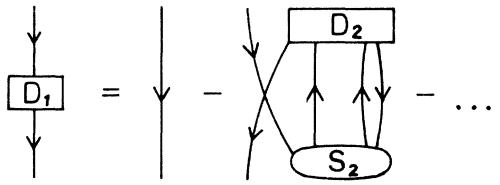
$$\langle\mu_1\mu_2|D_2|\nu_1\nu_2\rangle=\langle\mu_1\mu_2|\nu_1\nu_2\rangle_A-\sum\langle\mu_1\lambda|D_2|\sigma_1\sigma_2\rangle A_{\nu}(\langle\sigma_1\sigma_2|S_2|\nu_1\lambda\rangle\langle\mu_2|\nu_2\rangle)$$
$$-\sum\langle\lambda\mu_2|D_2|\sigma_1\sigma_2\rangle A_{\nu}(\langle\sigma_1\sigma_2|S_2|\lambda\nu_2\rangle\langle\mu_1|\nu_1\rangle)+\frac{1}{2}\sum\langle\mu_1\mu_2|D_2|\sigma_1\sigma_2\rangle\langle\sigma_1\sigma_2|S_2|\nu_1\nu_2\rangle_A+\cdots, \tag{4.16c}$$

$$\langle\mu_1\mu_2\mu_3|D_3|\nu_1\nu_2\rho_3\rangle=A_{\mu}(\langle\mu_1\mu_2|\nu_1\nu_2\rangle\langle\mu_3|D_1|\rho_3\rangle)+\cdots. \tag{4.16d}$$

The diagrammatic representation of (4.16) is given in Fig. 5. For the higher terms we refer the reader to Ref. 14.

It is seen that the terms in Figs. 2, 3, and 5 are now all related to the nondiagonal elements of the two-body density in Fig. 4. Thus we obtain a solvable coupled system of equations for the one- and two-body density matrix which, according to Ref. 14, satisfies conditions (i) and (ii) and moreover is equivalent to FBHF(3) calculations in the sense explained after writing conditions (i)–(iii).

In our first calculations reported in this paper we neglected the second term on the right hand side of Fig. 3. $\langle S_3\rangle$ is hard to calculate even if the solution of the Bethe-Faddeev equation is known. Note also that all the terms neglected here and in the other approximations contain expressions like $\langle S_n\rangle\langle S_m\rangle$ $(n+m\geq 5)$ and $\langle S_n\rangle\langle\chi_m\rangle$ $(m\geq 4)$. We now see



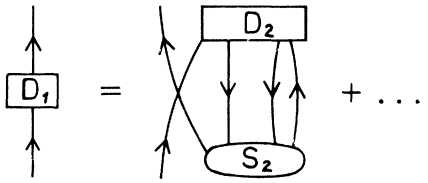


FIG. 2. Graphical representation of the Eq. (4.10).

that inserting Fig. 5(a) into Fig. 3 gives

$$\langle \rho | D_1 | \nu \rangle = 0 \Leftrightarrow \langle \psi | a_\nu^\dagger a_\nu | \psi \rangle = \max . \tag{4.17}$$

Thus, in this approximation we also fulfill, in addition to (4.4), the natural-orbital condition.[6,10] Also Fig. 5(d) is zero so that we are left in Fig. 4 with the first term on the right hand side. Inserting Fig. 5(c) into Fig. 4 we get Fig. 6. The second and third terms on the right hand side are clearly occupation probability insertions of the usual kind whereas the last term is a correction term.

For the true occupation probability defined by

$$\langle \nu | \kappa_2 | \nu \rangle = \sum_{\nu_1} \langle \nu_1 \nu | D_2 S_2 | \nu_1 \nu \rangle \tag{4.18a}$$

we get the approximation

$$\langle \nu | \kappa_2 | \nu \rangle \approx \frac{\langle \nu | \kappa | \nu \rangle}{1 + 2\langle \nu | \kappa | \nu \rangle} \tag{4.18b}$$

by multiplying $\langle S_2 \rangle$ on top of Fig. 6 and neglecting

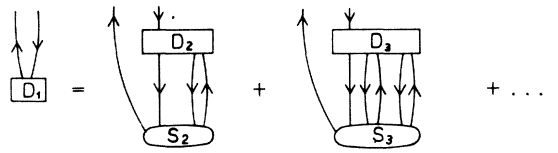


FIG. 3. Graphical representation of (4.13).

the term given by Fig. 6(d). Our average one-body occupation probability in this approximation is thus

$$\frac{1}{A} \sum_\nu \langle \nu | D_1 | \nu \rangle = 1 - \frac{1}{A} \sum_\nu \langle \nu | \kappa_2 | \nu \rangle \approx 1 - \kappa + 2\kappa^2 - 4\kappa^3 + 8\kappa^4 - \cdots . \tag{4.19a}$$

whereas Brandow[16] claims that it is

$$1 - \kappa + 2\kappa^2 - 5\kappa^3 + 11\kappa^4 - \cdots . \tag{4.19b}$$

The difference arises because not as many hole-line insertions are taken into account in our approximation as in Brandow's approach. It would not be hard for us to take them into account by expanding Fig. 5(c) further (compare Ref. 14). But in particular condition (ii) for the two-body density would then be violated. In Fig. 7 we give the contribution to the trace according to the basic expansion (4.15) using Figs. 6 and 5(b) and the definitions [(4.3(b) and (4.3c)] of $\langle \chi_2 \rangle$ and $\langle \chi_3 \rangle$. It is seen that the contributions from $\langle D_2 S_2 \rangle$ and $\langle D_3 \chi_3 \rangle$ cancel. Consequently, taking into account higher-order terms in (4.19a), we have to introduce higher $\langle \chi_n \rangle$ to fulfill condition (ii). Evidently our condition (ii) insures that particles and holes are treated to some extent symmetrically in our density matrices.

Using our expansion we may evaluate the matrix such that only Fig. 6 and Eq. (4.18a) have to be used in the calculation. We get from the Eqs. (3.9) and (4.15)

$$C_{\alpha\beta} = \langle \alpha | T D_1 | \beta \rangle + \sum_{\nu_1 \nu_2 \alpha_2} \langle \nu_1 \nu_2 | D_2 | \beta \alpha_2 \rangle \langle \alpha \alpha_2 | V \chi_2 | \nu_1 \nu_2 \rangle_A + \frac{1}{2} \sum_{\nu_1 \nu_2 \nu_3 \rho_3 \alpha_2} \langle \nu_1 \nu_2 \nu_3 | D_3 | \beta \alpha_2 \rho_3 \rangle \langle \alpha \alpha_2 \rho_3 | V_{12} \chi_3^{(12)} | \nu_1 \nu_2 \nu_3 \rangle_A + \cdots \tag{4.20a}$$

and using (4.16) the result

$$C_{\alpha\nu} = \langle \alpha | T D_1 | \nu \rangle + \sum_{\nu' \mu_2} \langle \alpha \mu_2 | V \chi_2 | \nu' \mu_2 \rangle_A \langle \nu' | D_1 | \nu \rangle - \sum_{\mu_2 \nu_2} \langle \alpha \mu_2 | V \chi_2 | \nu \nu_2 \rangle_A \langle \nu_2 | \kappa_2 | \mu_2 \rangle + \frac{1}{2} \sum_{\nu_i \mu_2} \langle \nu_1 \nu_2 | D_2 S_2 | \nu \mu_2 \rangle \langle \alpha \mu_2 | V \chi_2 | \nu_1 \nu_2 \rangle_A + \frac{1}{2} \sum_{\nu_i \rho_i} \langle \nu_2 \nu_3 | D_2 | \rho_2 \rho_3 \rangle \langle \alpha \rho_2 \rho_3 | V_{12} \chi_3^{(12)} | \nu \nu_2 \nu_3 \rangle_A \tag{4.20b}$$

and

$$C_{\alpha\rho}=\langle\alpha|TD_1|\rho\rangle+\frac{1}{2}\sum_{\nu_1\rho_2}\langle\nu_1\nu_2|D_2|\rho\rho_2\rangle\langle\alpha\rho_2|V\chi_2|\nu_1\nu_2\rangle_A$$

$$-\frac{1}{2}\sum_{\nu_2\nu\rho_3}\langle\nu_2\nu_3|D_2|\rho\rho_3\rangle\langle\alpha\nu\rho_3|V_{12}\chi_3^{(12)}|\nu\nu_2\nu_3\rangle_A. \tag{4.20c}$$

The interaction part C^V of $C_{\alpha\nu}$ and $C_{\alpha\rho}$ is given diagrammatically in Fig. 8.

In our first calculations we solve the equation of motion (3.7) only in a one-dimensional subspace (compare Ref. 4). We obtain from (3.7) and (4.20b)

$$\epsilon_{\hat{B},\nu}=\frac{C_{\nu\nu}}{\langle\nu|D_1|\nu\rangle}=\langle\nu|T|\nu\rangle+\sum_{\mu}\langle\nu\mu|V\chi_2|\nu\mu\rangle_A \tag{4.21a}$$

$$+\sum_{\mu_2\nu_2}\frac{\langle\nu\mu_2|V\chi_2|\nu\nu_2\rangle_A\langle\nu_2|\kappa_2|\mu_2\rangle}{1-\langle\nu|\kappa_2|\nu\rangle} \tag{4.21b}$$

$$+\frac{1}{2}\sum_{\nu_1\nu_2\mu_2}\frac{\langle\nu_1\nu_2|D_2S_2|\nu\mu_2\rangle\langle\nu\mu_2|V\chi_2|\nu_1\nu_2\rangle_A}{1-\langle\nu|\kappa_2|\nu\rangle} \tag{4.21c}$$

$$+\frac{1}{2}\sum_{\nu_2\nu_3\rho_2\rho_3}\frac{\langle\nu_2\nu_3|D_2|\rho_2\rho_3\rangle\langle\nu\rho_2\rho_3|V_{12}\chi_3^{(12)}|\nu\nu_2\nu_3\rangle_A}{1-\langle\nu|\kappa_2|\nu\rangle}. \tag{4.21d}$$

The first term on the right hand side is then the usual Brueckner-Hartree-Fock energy

$$h_\nu=\langle\nu|T|\nu\rangle+\sum_{\mu}\langle\nu\mu|V\chi_2|\nu\mu\rangle_A. \tag{4.22}$$

It is seen that the corrections due to the other terms will depend sensitively on the value of $\langle\nu|\kappa_2|\nu\rangle$, which in turn is quite different from the usual κ. The leading diagrams of the four interaction terms of (4.21) are given in Fig. 9, where Fig. 9(b) refers to the first, Fig. 9(c) to the second, and Figs. 9(d) and (e) to the third "correction term." (4.21b) is the "true renormalization term" for one-hole states, (4.21c) a correction originating from "hole-hole ladders," and (4.21d) is a part of the three-particle effect; another one is calculated in the FBHF(3) approximation (Fig. 9).

For ^{4}He and ^{16}O the matrix elements $\langle\nu|\kappa_2|\nu\rangle$ are diagonal for trivial reasons and the diagonal elements are nearly the same for all ν as we shall see in Sec. VI. The term (4.21b) is therefore given by

$$(4.21b)\approx -U_\nu\frac{\bar{\kappa}_2}{1-\bar{\kappa}_2}$$

where U_ν is the self-consistent BHF potential defined by

$$U_\nu=\sum_{\mu}\langle\nu,\mu|V\chi_2|\nu\mu\rangle_A \tag{4.22}$$

and $\bar{\kappa}_2$ the mean occupation probability defined by

$$\bar{\kappa}_2=\frac{1}{A}\sum_{\nu}\langle\nu|\kappa_2|\nu\rangle. \tag{4.23}$$

Note that the true "renormalization term" (4.21b) is given by neither $(-U\kappa)$ nor $(-U\bar{\kappa}_2)$ [compare (7.4a)]. In fact it is smaller than the former and larger than the latter term. In the second-order approximation the following equations are valid:

$$-U\frac{\bar{\kappa}_2}{1-\bar{\kappa}_2}=-U\kappa(1-\kappa), \tag{4.24a}$$

$$-U\bar{\kappa}_2=-U\kappa(1-2\kappa), \tag{4.24b}$$

and therefore

$$(4.21b)\approx -U\tfrac{1}{2}(\kappa+\bar{\kappa}_2). \tag{4.24c}$$

In an alternative treatment of one-hole states in the expS formalism, equations for the $A-1$ nucleus are derived in a model space treatment[17] (the iterated equations are equivalent to degenerate perturbation theory). Then occupation probabilities are not introduced explicitly. We are quite sure that in the calculation of closed-shell nuclei it is not useful to introduce them (compare the discussion in Refs. 10 and 13). However, in the calculation of the $A-1$ nucleus the knowledge about the A-particle closed-shell nucleus is used and the situation is different. For this reason we are not sure which theory is preferable. In any case, in order to compare the two formalisms our formulation has to be developed further and the total wave function (2.4) of the $(A-1)$-particle nucleus

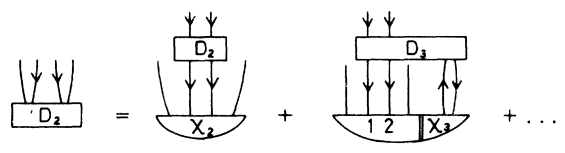


FIG. 4. The basic expansion (4.15) for occupied states $|\beta_1\rangle$, $|\beta_2\rangle$.

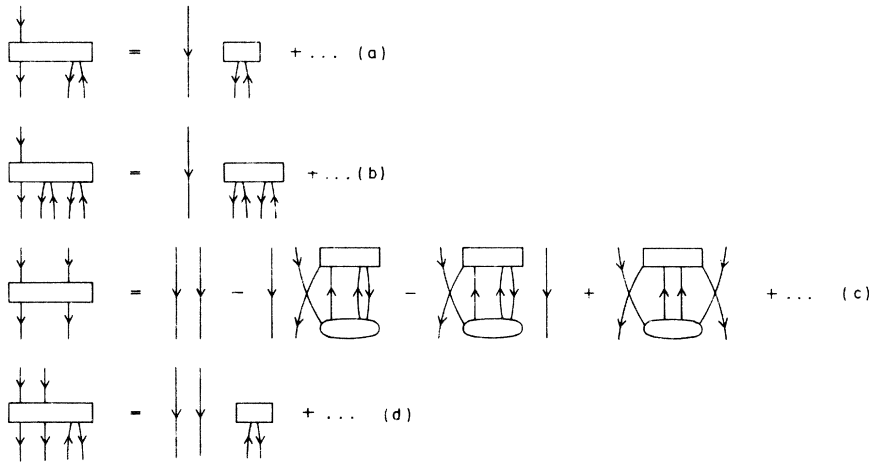


FIG. 5. Graphical representation of (4.16).

has to be included. Work in this direction is under way.

V. COUPLING OF THE ONE-HOLE STATES TO EXCITED CORE STATES

In this section we shall briefly discuss the connection between centroids and the exact eigenstates of ^{15}N and ^{3}H. If the excited states of the double-magic core nucleus are known, we can use the expansion (2.4) and, instead of (3.7) the analogous formula

$$\sum_{\alpha}\sum_{s=0}^{S_n}[-C^{S's}_{\alpha'\alpha}-(E_B-E_0)D^{S's}_{\alpha'\alpha}](\beta^S_\alpha)^*=0\,, \qquad (5.1)$$

with

$$-C^{S's}_{\alpha'\alpha}=\langle\psi_S|a^\dagger_\alpha[H,a_{\alpha'}]|\psi_{S'}\rangle + \langle\psi_S|a^\dagger_\alpha a_{\alpha'}|\psi_{S'}\rangle(E_S-E_0)\,, \qquad (5.2)$$

$$D^{S's}_{\alpha'\alpha}=\langle\psi_s|a^\dagger_\alpha a_{\alpha'}|\psi_{S'}\rangle\,.$$

It is easy to see that the additional terms originating from coupling the one-hole state to ph excitations of the core are of the kind in Fig. 10. It is clear that the coupling strength of the most simple terms is given by $\langle V\chi_2\rangle$ matrix elements (the G matrix) and is therefore large. On the other hand, the energy of the particle-hole excitations of the core is large in the case of ^{16}O and ^{4}He and one may therefore employ perturbation theory: The Pauli rearrangement term [Fig. 10(a)] yields the correct order of magnitude. This is, in general, not true for heavier double-magic nuclei and especially not true for the $1s$ state of ^{15}N because the energy of the latter state is approximately the energy of a p state plus the energy of a p-h pair. Our results show that the centroid energy defined by (3.18) does not considerably depend on whether we use for $|\alpha\rangle$ the natural orbital state or the state $|\Phi_{\hat{\beta}}\rangle$ or an empirical shell-model state [we shall discuss this point in more detail in Sec. VIII, compare (8.1)]. There is, however, another point which is much more important: Experimentalists do not average over all states $|\psi_B\rangle$ if they determine the centroid energy defined by (2.6). We now discuss this point for the example of ^{15}N.

From Ref. 18 the spectroscopic factors are known for states with excitation energy up to 11 MeV, corresponding to about 23 MeV separation energy. The $p^{3/2}$ state of ^{15}N is "split" into three states with appreciable strength because the low-lying excited ^{16}O states, especially the four-particle–four-hole states, couple to the one-hole state. From the fact that this splitting is not very strong we may conclude that the corresponding "coupling strength" is rather small. Therefore, high-lying four-particle–four-hole states will be rather irrelevant for the centroid energy given by (3.18); we know that the one-particle–one-hole states have a large "coupling strength" approxi-

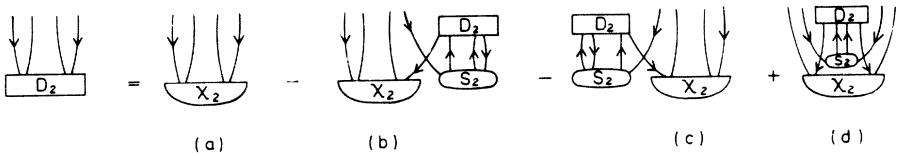


FIG. 6. The resulting inhomogeneous equation for the matrix elements $\langle\alpha_1\alpha_2|D_2|\nu_1\nu_2\rangle$.

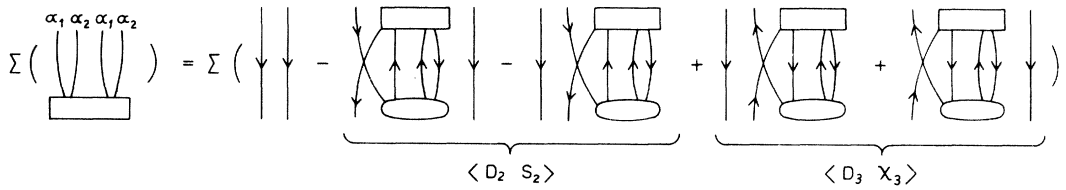


FIG. 7. The conservation of the trace of the two-particle density matrix.

mately given by the G matrix (Fig. 10). Nevertheless, the influence of this coupling may be calculated in perturbation theory because the separation energy of the (2h-1p) states is about 43 MeV or more, compared with about 15 MeV of the one-hole states. From the homogeneous Dyson equation the formula[19]

$$\langle \nu | \epsilon_{\hat{B},\nu} + R(\omega) | \nu' \rangle = \epsilon_i(\omega)\delta_{\nu\nu'}, \quad \epsilon_i(\omega) = \omega \tag{5.3}$$

follows with

$$\langle \nu | R(\omega) | \nu' \rangle = \sum_{n=1}^{\infty} \sum_{\mu\nu_1\rho_1} \frac{\langle \nu\rho_1 | G | \mu\nu_1 \rangle \langle \mu\nu_1 | G | \nu'\rho_1 \rangle}{\omega - \epsilon_{\hat{B},\mu} + 2n\hbar\omega_{\text{osc}}},$$

$$n = n(\nu_1, \rho_1), \quad \hbar\omega_{\text{osc}} = 14 \text{ MeV}.$$

(5.3) yields the energies of the fragmented states. $R(\omega)$ is evidently the contribution to the self-energy originating from the "Pauli rearrangement" term shown in Fig. 10(a). The corresponding single-hole strengths of the fragmented states are given by[19]

$$S_i(\nu) = \frac{1}{1 - d/d\omega\, R_{\nu\nu}(\omega)_{\epsilon_i}}. \tag{5.4}$$

In the ^{4}He nucleus the excited states have an excitation energy of more than 20 MeV. The coupling to complicated states will probably be rather weak, but the coupling to particle-hole states is important for the ^{3}H and ^{3}He ground-state energies. Again, we have approximated this effect by (5.3) using the Pauli rearrangement term for $R(\omega)$.

As mentioned above, we only claim to give here the correct order of magnitude of the coupling of one-hole states to the excited core states. A treatment avoiding perturbation theory is in preparation.

VI. PRELIMINARY RESULTS

In this section we report some numerical results obtained within a one-dimensional subspace. They are *preliminary* insofar as the approximate center-of-mass correction given in Appendix C by (C5) is used and the energies $\epsilon_{\hat{B},\nu}$ defined by (4.21) are calculated instead of the eigenvalues $\epsilon_{\hat{B}}$ of (3.7); the Coulomb correction, i.e., the difference for proton or neutron levels is taken from experiment. We performed calculations for four different NN interactions: These are Hamada-Johnston[20] (HJ), Reid soft core[21] (RSC), de Tourreil-Sprung supersoft core[22] (SSCB), and RSC plus the effective two-body force obtained from a two-pion exchange three-body force by Blatt and McKellar. The force of Ref. 23 is in error[23a] due to a numerical mistake, but our results indicate qualitatively the effect of a three-body force. Also different approximations for the ground state of the double closed-shell nucleus were used.

In Table I we give results for ^{3}H. In the third column we give the BHF energies h_ν used in the determination of the ^{4}He ground-state wave function.[8-10] This is the leading term of (4.21). In this equation there are three correction terms: the renormalization contribution, the hole-hole contribution, and the contribution from the three-particle Bethe-Faddeev amplitude. The last one is, of course, equal to zero in a GBHF-type calculation. The size of these terms depends critically upon the value of κ_2 defined by (4.18a). These values are given in the fourth column of Table I. They depend strongly on the NN interaction used as well as on the approximation to the closed-shell

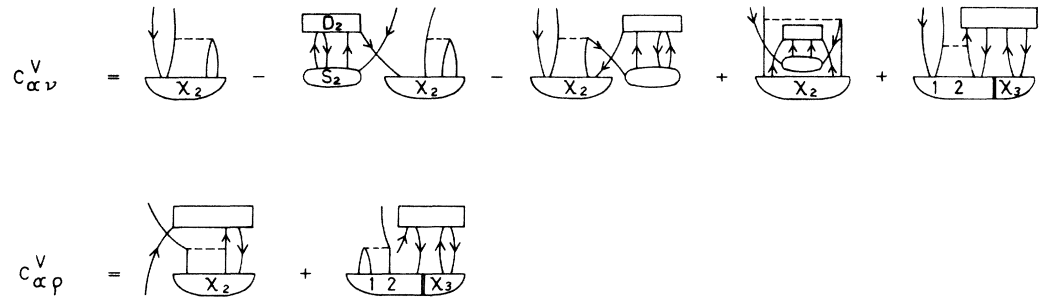


FIG. 8. The interaction part of the operator C.

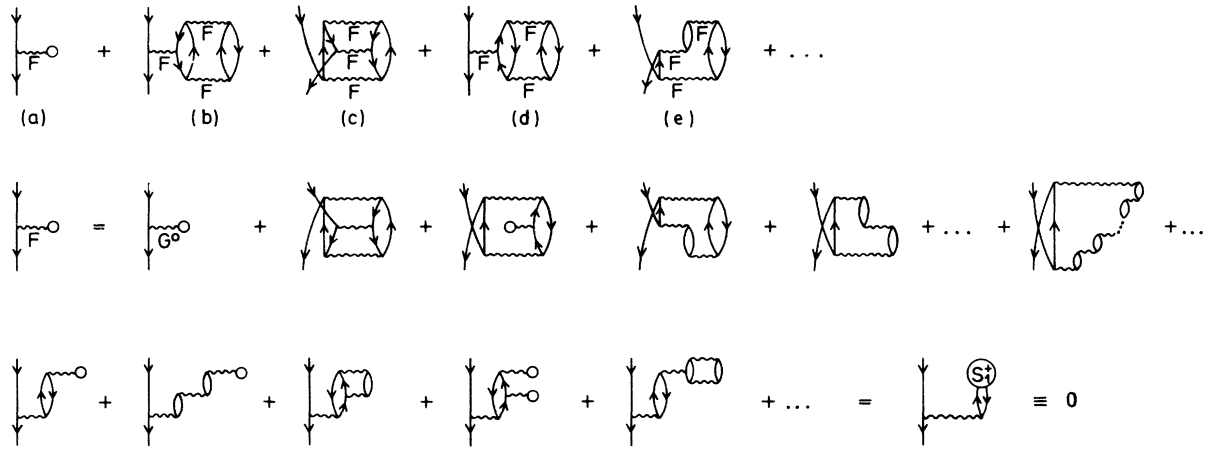


FIG. 9. Upper line: the leading diagrams of (4.21). Second line: some terms of the BHF energy h_ν calculated in FBHF(3) and given here in terms of the G^0 matrix. Third line: sum of diagrams which disappear because of (4.4). The wavy lines which are not denoted by F represent the (antisymmetrized) G^0 matrix.

wave function. The latter dependence is due to higher-order correlations which increase the value of κ_2.

The first of the correction terms in (4.21) depends on the self-consistent BHF potential

$$\langle \nu | U | \nu \rangle = \sum_{\nu_2} \langle \nu\nu_2 | V\chi_2 | \nu\nu_2 \rangle_A$$

whose values are given in the fifth column. The next three columns give these three correction terms from Eqs. (4.21). It is seen that the renormalization term is the largest one, partially being cancelled by the hole-hole term. The renormalization is further reduced by the three-particle contribution. This is quite in line with the corresponding contributions to the two-particle (Bethe-Goldstone) equation of the expS hierarchy (see Refs. 9 and 10). The leading diagrams of these three terms are given in Figs. 9(b), 9(c), and 9(d) and (e), respectively. Note that *all* the diagrams of Fig. 9 and many more complicated ones are really taken into account in our calculation. The next four columns of Table I give the total values for (4.21), the c.m. [from Eq. (C6)] and Coulomb corrections, and the total result for the centroid energy $\epsilon_{\hat{B},\nu}$. The values show a trend which was to be expected: Those potentials yielding small binding energies for the closed-shell nucleus yield small separation energies as well, and vice versa. The same is true for the transition from the simple GBHF approximation of the closed-shell wave function to the more sophisticated FBHF(3) approximation. To compare these results with experimental values, i.e., the separation energy, we have to add the Pauli rearrangement term, taking into account the coupling to excited particle-hole states of the core as described in Sec. V. Instead of the separation energy we give in the next column the triton binding energy itself which we obtain from the separation energy and the ^{4}He energy given in column 15. This calculation of the triton energy should be considered to be a test for our approximate c.m. correction. [From our results we conclude that the c.m. correction given by (C6) probably is sufficiently accurate for the calculation of ^{16}O and ^{40}Ca separation energies because it is much smaller for these heavier nuclei.] The last two columns give the binding energy per particle and the charge radius for the double closed-shell nucleus ^{4}He.

Table II gives the corresponding results for ^{15}N in the GBHF approximation, i.e., without inclusion of the three-body correlations. The correction terms were calculated with an average value for κ_2. The individual values as well as the averages are given in the fourth column. It is seen that the use of the average is very well justified. The same trends as in Table I are observed.

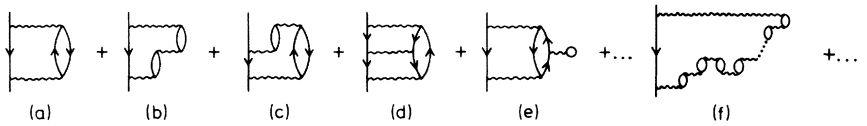


FIG. 10. Diagrams representing the coupling of p-h states to the one-hole state; compare the text.

TABLE I. GBHF and FBHF(3) calculations for ^{3}H. The values are given in MeV.

Potential	Approx.	$\frac{1}{2}[h_\nu(p)+h_\nu(n)]$	κ_2	U	(4.21b)	(4.21c)	(4.21d)	$\epsilon_{\hat{B},\nu}$	(C6)	$\frac{1}{2}E_{\text{Coul}}$	$\epsilon_{\hat{B},\nu}$(corr.,p)	Eq. (5.3)	E (^{3}H)	^{4}He E_0/A	^{4}He r_c (fm)
RSC	GBHF	−20.210	0.09552	−30.89	3.262	−1.195		−18.14	2.95	0.38	−14.8			−4.76	1.77
RSC	FBHF(3)	−23.251	0.11670	−35.56	4.672	−1.697	−0.948	−21.22	3.47	0.38	−17.4	+1.6	−6.1	−5.47	1.64
RSC + V_{McK}	GBHF	−25.171	0.10831	−37.00	4.494	−1.707		−22.38	3.32	0.38	−18.7			−6.67	1.67
RSC + V_{McK}	FBHF(3)	−28.538	0.12506	−41.93	5.994	−2.256	−1.195	−26.00	3.83	0.38	−21.8	+2.4	−10.9	−7.57	1.57
HJ	GBHF	−17.890	0.11034	−27.31	3.387	−1.105		−15.61	2.65	0.38	−12.6			−4.23	1.88
HJ	FBHF(3)	−20.749	0.12998	−31.90	4.765	−1.548	−0.955	−18.49	3.20	0.38	−14.9	1.0	−5.3	−4.80	1.73
SSCB	GBHF	−23.442	0.05783	−35.30	2.167	−0.836		−22.11	3.15	0.38	−18.6			−5.79	1.68
SSCB	FBHF(3)	−25.637	0.06913	−38.51	2.860	−1.095	−0.667	−24.54	3.46	0.38	−20.7	+1.8	−6.6	−6.38	1.61
												Exp:	−8.48	−7.07	1.59
															−1.67

TABLE II. GBHF calculations for ^{15}N.

Potential	State	$\frac{1}{2}[h_\nu(p)+h_\nu(n)]$	$\langle\nu\mid\kappa_2\mid\nu\rangle$	$\langle\nu\mid U\mid\nu\rangle$	(4.21b)	(4.21c)	$\epsilon_{\hat{B},\nu}$	(C6)	$\frac{1}{2}E_{\text{Coul}}$	$\epsilon_{\hat{B},\nu}$(corr.,p)	^{16}O E_0/A	^{16}O r_c (fm)
RSC	$s_{1/2}$	−39.40	0.0921	−49.5	4.70	−0.70	−35.40	1.06	(1.6)	−32.7	−4.45	2.600
	$p_{3/2}$	−20.01	0.0825	−36.9	3.47	−0.48	−17.02	1.02	1.7	−14.3		
	$p_{1/2}$	−16.63	0.0882	−33.2	3.14	−0.50	−13.98	1.03	1.8	−11.15		
			$\kappa_2 = 0.0863$									
RSC + V_{McK}	$s_{1/2}$	−46.56	0.1016	−57.3	6.11	−0.95	−41.40	1.17	(1.6)	−38.6	−6.47	2.499
	$p_{3/2}$	−25.05	0.0915	−43.5	4.58	−0.66	−21.13	1.12	1.7	−18.3		
	$p_{1/2}$	−20.83	0.0981	−38.9	4.13	−0.68	−17.38	1.13	1.8	−14.5		
			$\kappa_2 = 0.0957$									
HJ	$s_{1/2}$	−32.35	0.1054	−40.8	4.48	−0.67	−28.54	0.92	(1.6)	−26.0	−3.41	2.809
	$p_{3/2}$	−16.12	0.0943	−30.5	3.31	−0.48	−13.29	0.88	1.7	−10.7		
	$p_{1/2}$	−13.93	0.0993	−28.0	3.06	−0.49	−11.36	0.88	1.8	−8.7		
			$\kappa_2 = 0.0984$									
SSCB	$s_{1/2}$	−51.58	0.0563	−63.8	3.68	−0.56	−48.47	1.23	(1.6)	−45.6	−5.89	2.387
	$p_{3/2}$	−27.04	0.0521	−47.5	2.72	−0.38	−24.70	1.19	1.7	−21.8		
	$p_{1/2}$	−20.64	0.0569	−40.3	2.32	−0.37	−18.69	1.20	1.8	−15.7		
			$\kappa_2 = 0.0543$									

Table III gives the ^{15}N results with FBHF(3) wave functions. The averaged value for κ_2 has been used. The values for κ_2 as well as their average is given in the fourth column. Again the averaging is very well justified. The values are larger than those given in Table II because of the additional correlations taken into account. In the language of BHF theory, this reflects the influence of the particle potential taken into account now as part of the three-body Bethe-Faddeev amplitude. For the same reason the BHF single-particle (s.p.) energies are more attractive than in GBHF, as is the s.p. potential U. In addition we have a contribution from the three-body Bethe-Faddeev amplitude (column 8). Since the renormalization term is larger, the total results for the 1p holes are only about 1 MeV more attractive than in GBHF (column 9). The values given are averages over proton- and neutron-hole states, i.e., the average separation energy for ^{15}O and ^{15}N. The correction from the c.m. motion is given in column 10. To obtain the ^{15}N separation energies we have to add $\frac{1}{2}$ of the Coulomb energy. We take this correction from experiment and give the numerical values in the 11th column. Thus we obtain the centroid energy given in column 12. To compare with experimental values[18] where the centroid is taken over the low-lying states only (up to about 11 MeV) we have to eliminate the influence from the high-lying two-hole–one-particle states. This is done in perturbation theory as described in Sec. VI. The resulting Pauli rearrangement is given in column 13. The last two columns give the ^{16}O binding energy and charge radius for comparison. The final results for the separation energies are given in Fig. 11 together with the experimental values.[18] The latter ones are given for the dominant states (Exp. 1) as well as for the centroids (Exp. 2).

From the Tables I–III one may draw the following conclusions:

(i) As was to be expected, the BHF energies are a very bad approximation to the separation energies. The BHF energies are purely theoretical quantities used in the description of the double closed-shell nucleus. They are introduced without aiming to describe hole states, i.e., neighboring nuclei.[24]

(ii) The separation energies as well as the spin-orbit splittings ($p_{1/2}$ vs $p_{3/2}$) are too small in absolute magnitude for potentials yielding too small a binding energy for ^{16}O; compare the second to the last column of Table III. With increasing binding for ^{16}O the separation energy increases as well as the spin-orbit splitting. For the SSCB potential, which almost yields the correct ^{16}O binding energy, we obtain separation energies in

TABLE III. FBHF(3) calculations for ^{15}N. Compare also Fig. 11.

Potential	State	$\frac{1}{2}[h_\nu(p)+h_\nu(n)]$	$\langle\nu\vert\kappa_2\vert\nu\rangle$	$\langle\nu\vert U\vert\nu\rangle$	(4.21b)	(4.21c)	(4.21d)	$\epsilon_{\beta,\nu}$	(C6)	$\frac{1}{2}E_{\text{Coul}}$	$\epsilon_{\beta,\nu}(\text{corr.},p)$	Eq. (5.3)	^{16}O E_0/A	^{16}O r_c (fm)
RSC	$s_{1/2}$	−41.09	0.1023	−51.4	5.75	−0.97	−0.88	−37.18	1.10	(1.6)	−34.5			
	$p_{3/2}$	−21.18	0.0962	−38.5	4.29	−0.67	−0.46	−18.03	1.06	1.7	−15.3	+3.1	−4.90	2.572
	$p_{1/2}$	−17.77	0.1074	−34.8	3.91	−0.70	−0.58	−15.13	1.08	1.8	−12.25	+3.9		
			$\kappa_2=0.1005$											
RSC + V_{MeK}	$s_{1/2}$	−48.32	0.1127	−59.3	7.43	−1.33	−1.13	−43.35	1.21	(1.6)	−40.5			
	$p_{3/2}$	−26.32	0.1065	−45.1	5.61	−0.92	−0.58	−22.21	1.16	1.7	−19.35	+4.3	−7.02	2.482
	$p_{1/2}$	−22.15	0.1192	−40.5	5.12	−0.96	−0.72	−18.71	1.18	1.8	−15.7	+5.3		
			$\kappa_2=0.1112$											
HJ	$s_{1/2}$	−33.62	0.1148	−42.3	5.36	−0.91	−0.64	−29.80	0.95	(1.6)	−27.25			
	$p_{3/2}$	−16.90	0.1082	−31.6	3.97	−0.65	−0.34	−13.92	0.91	1.7	−11.3	+2.2	−3.69	2.780
	$p_{1/2}$	−14.61	0.1177	−29.0	3.69	−0.67	−0.37	−12.00	0.92	1.8	−9.3	+2.8		
			$\kappa_2=0.1122$											
SSCB	$s_{1/2}$	−53.13	0.0639	−65.5	4.52	−0.78	−0.88	−50.27	1.26	(1.6)	−47.4			
	$p_{3/2}$	−28.20	0.0616	−49.0	3.37	−0.52	−0.47	−25.83	1.22	1.7	−22.9	+4.7	−7.17	2.372
	$p_{1/2}$	−21.82	0.0711	−41.8	2.90	−0.52	−0.61	−20.04	1.24	1.8	−17.0	+5.3		
			$\kappa_2=0.0645$									Exp.:	−7.96	2.65
														−2.73

excellent agreement with the experimental values. Thus it is clearly seen that the old argument that energy differences may be described well by an prescription yielding wrong absolute values for, e.g., the ground-state energy, is not justified. On the contrary, a prescription yielding too small values for the ground-state energy will yield too small absolute values for the excitation energies too. Thus the level spacing comes out too small as well. This could easily be understood by introducing a "strength multiplier" greater than unity to the potential. Thereby the ground-state energy as well as all other energies will be enlarged. Thus the same holds true for energy differences.

We warn the reader, however, not to draw the conclusion that the SSCB potential yields a reasonable description of nuclei. For the ground state of ^{16}O the energy is described well, but the charge radius and charge form factor are reproduced quite badly.[25] Also a preliminary calculation for ^{40}Ca shows that this potential overbinds that nucleus with a correspondingly much too small radius and much too high central density. This is why the separation energies come out much too large in absolute magnitude; compare Table IV.

In Table V we give some results for the usual BHF method in comparison with our GBHF method. The difference is essentially due to the hole-hole ladders taken into account in GBHF. It is seen that the hole-hole ladders are of the same importance as the three-body Bethe-Faddeev contributions; compare Tables II and III.

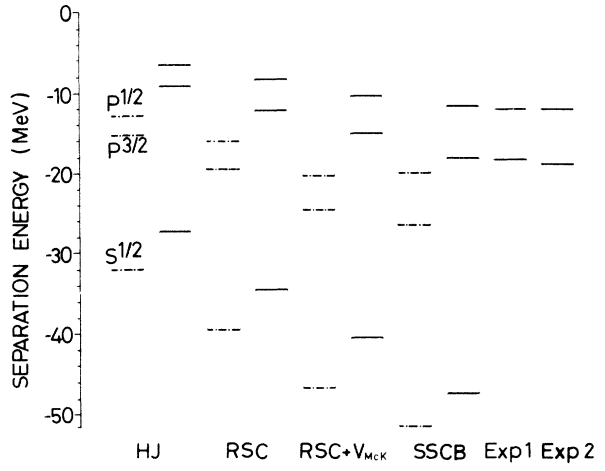


FIG. 11. The separation energies for the ^{15}N states. The dot-dash lines denote the BHF energies in the FBHF(3) approximation (sum of the third and the eleventh column of Table III). The full lines give the results of (4.21) including c.m. and Coulomb corrections and—for the p states—the correction originating from the solution of (5.3). Further explanation is in the text.

TABLE IV. GBHF calculations for ^{40}Ca with the SSCB potential. For ^{40}Ca we obtained for the energy $E_0/A = -8.77$ MeV (exp.: -8.55 MeV), and for the charge radius $r_c = 2.92$ (fm) [exp.: 3.44–3.47 (fm)]. Results for other potentials may be found in Refs. 10 and 25.

State	$\frac{1}{2}[h_\nu(p)+h_\nu(n)]$	$\epsilon_{\hat{B},\nu}$(corr., n)	Exp.: Dominant states (n)
$1s_{1/2}$	−76.6	−74.3	(−50.0)
$p_{3/2}$	−54.2	−52.6	(−30.0)
$p_{1/2}$	−47.3	−46.0	−27.0
$d_{5/2}$	−32.7	−31.9	−21.9
$2s_{1/2}$	−26.3	−26.2	−18.2
$d_{3/2}$	−21.9	−22.0	−15.6

The separation energies $\epsilon^{(1)}_{\hat{B}\nu}$ of Table V were calculated from (4.21) taking into account only terms up to the order $\langle S_2\rangle^2$ in the correction terms. Comparing the GBHF results of Table V with those of Table II it is seen that the higher orders are by no means negligible. The importance of higher-order terms may also be observed in Table VI where we compare the values for the Bethe parameter κ with the values for κ_2 where $1-\langle\nu|\kappa_2|\nu\rangle$ is the occupation probability for the state ν. Thus it is clearly seen that the low-order prescription $1-\kappa$ for the occupation probabilities is a bad approximation! Instead the true occupation probabilities $1-\kappa_2$ have to be used, i.e., the higher orders of renormalization have to be taken into account.

As we have seen, Eq. (3.18) yields the energy of the centroid over *all* states; its strength is given by

$$\langle\alpha|D|\alpha\rangle = \sum_{B(A-1)} \langle\alpha|\Phi_B\rangle\langle\Phi_B|\alpha\rangle = \sum_{B(A-1)} S_\alpha(B)\,. \qquad (6.1)$$

Both the energy and the strength depend on $|\alpha\rangle$ but the values are very similar (up to 1%) if we take for $|\alpha\rangle$ a natural orbital, or the wave function $|\Phi_{\hat{B}}\rangle$, or an empirical shell-model wave function (com-

TABLE V. Comparison of BHF and GBHF calculations for ^{16}O. The values are averages over ^{15}N and ^{15}O separation energies.

Potential	State	BHF h_ν	BHF $\epsilon^{(1)}_{\hat{B},\nu}$	GBHF h_ν	GBHF $\epsilon^{(1)}_{\hat{B},\nu}$
RSC	$s_{1/2}$	−38.1	−31.7	−39.4	−33.7
	$p_{3/2}$	−19.2	−15.1	−20.0	−16.2
	$p_{1/2}$	−15.9	−12.0	−16.7	−13.0
HJ	$s_{1/2}$	−31.0	−24.2	−32.8	−26.6
	$p_{3/2}$	−15.3	−11.0	−16.3	−12.2
	$p_{1/2}$	−13.1	−9.05	−13.9	−9.9

TABLE VI. Comparison of $\bar{\kappa}_2$ and κ for the RSC potential.

Nucleus	$\bar{\kappa}_2$	κ
^{4}He	0.117	0.140
^{16}O	0.100	0.122

pare Sec. VIII). For the natural orbital centroids the strengths may be taken from the Tables I–III. They are about 10% less than one.

By the procedure described in Sec. V the centroid over all states is fragmented into a centroid over the low-lying states and some high-lying levels with very small strengths. The relative strengths are given by (5.4). Multiplying these with the factor (6.1) we obtained for ^{15}N and the RSC potential, one gets the results given in Fig. 12. The centroid over low-lying states is, of course, further fragmented by the coupling to the low-lying excited ^{16}O states. Combining the experimental relative strengths[18] 0.86, 0.07, and 0.07 of the low-lying ^{15}N states with our result one gets a strength of 0.72 for the dominant $p_{3/2}$ state in ^{15}N. For the $p_{1/2}$ state the coupling to low-lying ^{16}O states is found to be very weak in experiment: up to 11 MeV excitation energy there is only one state (the ground state) having an appreciable strength.[18] We obtained a strength of 0.82 for the centroid over the weakly excited states.

VII. COMPARISON WITH THE SHELL MODEL

In this section we compare the interaction part of the operator C with the shell-model potential and the wave function $\langle \vec{r}\,|\Phi_{\hat{B}}\rangle$ with the shell-model wave function. This discussion is continued in Sec. VIII.

In the following we denote the interaction part of the operator C by C^V. The Eq. (3.7) may then be written in the following way:

$$(T + C^V D_1^{-1} - \epsilon_{\hat{B}})\,|\Phi_{\hat{B}}\rangle = 0\,. \tag{7.1}$$

It is evident that the operator $C^V D_1^{-1}$ corresponds to the empirical shell-model potential. It is, however, not identical with a shell-model potential for three reasons:

(i) First, the operator $C^V D_1^{-1}$ is not Hermitian though it has a real spectrum as shown in Sec. III.
(ii) Secondly, it describes only one-hole states and no one-particle states.
(iii) Thirdly, it has a purely negative spectrum.

If the calculated C is Hermitian the operator $C^V D_1^{-1}$ is, up to a few percent, Hermitian in the subspace of occupied natural orbital states. This follows from the fact that the matrix elements $\langle\nu|D_1|\nu\rangle$ are given by (compare Table III)

$$\langle\nu|D_1|\nu\rangle = 1 - \langle\nu|\kappa_2|\nu\rangle \approx 1 - \bar{\kappa}_2 \tag{7.2}$$

so that TD_1 is Hermitian, and with TD_1 the operators C^V and $C^V D_1^{-1}$ are Hermitian too. This may also be seen from the diagrams of Fig. 9.

Hermitian expressions for $C^V D_1^{-1}$ may also be obtained in the following way: approximating C^V by its leading term, i.e., the $\langle D_2\rangle\langle V\chi_2\rangle$ term of (4.20a) and the matrix D_2 by

$$\langle\alpha_1\alpha_2|\,D_2|\,\alpha_1'\alpha_2'\rangle = \langle\alpha_1|\,D_1|\,\alpha_1'\rangle\langle\alpha_2|\,D_1|\alpha_2'\rangle - \langle\alpha_1|\,D_1|\,\alpha_2'\rangle\langle\alpha_2|\,D_1|\,\alpha_1'\rangle\,, \tag{7.3}$$

one obtains the "renormalized Hartree-Fock" expression[2]

$$\langle\alpha|\,C^V D_1^{-1}|\beta\rangle = \sum_{\nu_1\nu_2\alpha_2} \langle\alpha\alpha_2|V\chi_2|\beta\nu_2\rangle_A \langle\nu_2|\,D_1|\,\alpha_2\rangle\delta_{\nu_1\beta} \tag{7.4}$$

which is evidently Hermitian in the subspace of occupied states if $\langle V\chi_2\rangle$ is replaced by an Hermitian G matrix.[10] In this space one may also approximate (7.4) by

$$\langle\nu|\,C^V D_1^{-1}|\,\mu\rangle = \langle\nu|\,U|\,\mu\rangle(1-\bar{\kappa}_2)\,. \tag{7.4a}$$

One should compare this with (4.21) and (4.24c). Note, however, that for the nuclei we calculated (7.2) is much better fulfilled than (7.3) and (7.4).

We would like to warn the reader against a too simple Hermitianization procedure in the *complete* Hilbert space. If one would drop the restriction that $|\alpha\rangle$ and $|\beta\rangle$ belong to the occupied states one would obtain an Hermitian operator with a real but non-negative spectrum. This would not be a good approximation for hole states.

It has still to be shown that the functions $\langle\vec{r}|\Phi_{\hat{B}}\rangle$ have the form that one expects for shell-model wave functions. For simplicity we will show this for the case where only one occupied state exists for given j, π, and m (this is trivially fulfilled for ^{4}He, ^{16}O, and ^{40}Ca with the exception of the s states of ^{40}Ca). We denote the BHF state with these quantum numbers by $n=1$ because it is a natural orbital in our approximation. Now (3.14) may be written, using (3.13b), as

$$\sum_{n=1}^{\infty} \frac{|\langle n|\Phi_{\hat{B}}\rangle|^2}{\rho_n} S(\hat{B}) = \sum_{n=1}^{\infty} |\langle n|\Phi_{\hat{B}}\rangle|^2 \tag{7.5}$$

or

$$|\langle 1|\Phi_{\hat{B}}\rangle|^2\left(1 - \frac{S(\hat{B})}{\rho_1}\right) = \sum_{n=2}^{\infty} |\langle n|\Phi_{\hat{B}}\rangle|^2\left(\frac{S(\hat{B})}{\rho_n} - 1\right). \tag{7.5a}$$

From this equation we get

$$\frac{|\langle 1|\Phi_{\hat{B}}\rangle|^2}{\sum_{n=2}^{\infty}|\langle n|\Phi_{\hat{B}}\rangle|^2} \geq \left(\frac{S(\hat{B})}{\max_{n\geq 2}\rho_n} - 1\right)\left(1 - \frac{S(\hat{B})}{\rho_1}\right)^{-1}. \quad (7.6)$$

Preliminary results show that for an occupied state the strength $S(\hat{B})$ is, at any rate, greater than 0.6 and ρ_n smaller than 0.01 for $n \geq 2$. It follows that the quotient (7.6) is greater than 170, i.e.,

$$\frac{\langle 1|\Phi_{\hat{B}}\rangle}{(\langle\Phi_{\hat{B}}|\Phi_{\hat{B}}\rangle)^{1/2}} > 0.997, \quad (7.7)$$

and this is a very conservative estimate. It is well known that for light mass nuclei the empirical shell-model functions well resemble the single-

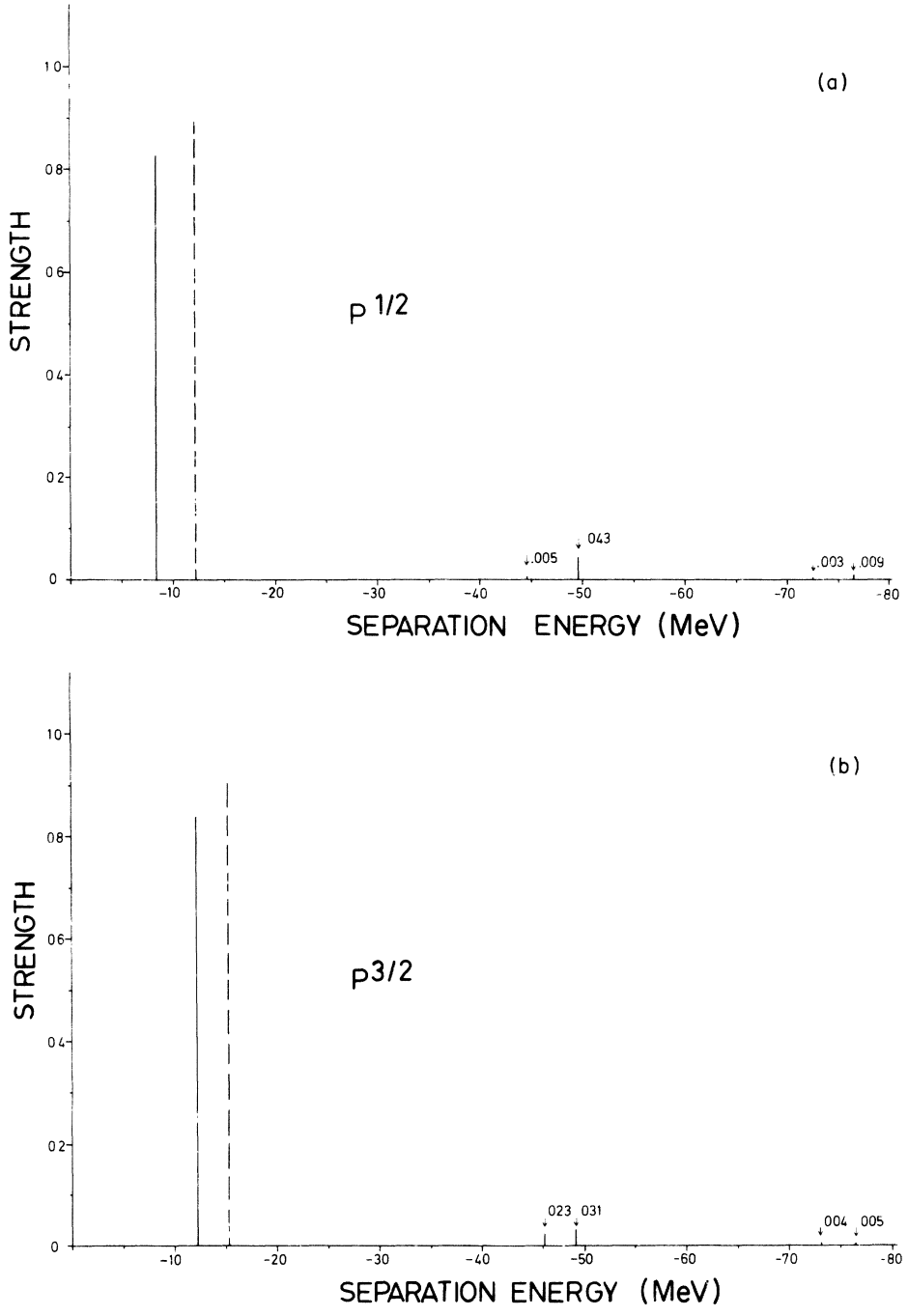


FIG. 12. The fragmentation of the p states of ^{15}N by the coupling of p-h states to the pure one-hole states. The calculation is performed with the RSC potential.

particle BHF functions and therewith also our functions $\Phi_{\hat{B}}(\vec{r})$. At the nuclear surface there may be, on the other hand, an appreciable difference between $\Phi_{\hat{B}}(\vec{r})$ and the BHF function (and between the Brueckner-Hartree-Fock and the shell-model function) even if the overlaps $\langle n|\Phi_{\hat{B}}\rangle$ are only a few percent or less for $n>1$.

If there are several occupied states to given j,π,m one can analogously show that the occupied states yield the overwhelming part of the right hand side of (7.5). From this and the approximate Hermiticity of $C^{V}D_1^{-1}$ in the subspace of occupied states it follows that the functions $\Phi_{\hat{B}_i}$ are approximately orthogonal; note also that the corresponding $(A-1)$-particle functions $|\psi_{\hat{B}_i}\rangle$ are exactly orthogonal.

We now discuss matrix elements of one-particle operators ${}^1O$. In the one-hole approximation they are given by

$$
\begin{aligned}
{}^1O_{\hat{B}\hat{A}} &= \langle\psi_{\hat{B}}|{}^1O|\psi_{\hat{A}}\rangle \\
&= \sum_{\alpha\alpha'\delta\delta'} \langle\psi_0|a_\delta^\dagger a_\alpha^\dagger a_{\alpha'} a_{\delta'}|\psi_0\rangle \beta_\delta^*(\hat{B})\,\beta_{\delta'}(\hat{A})\,{}^1O_{\alpha\alpha'}\,,
\end{aligned}
\tag{7.8}
$$

where

$$
\langle\psi_{\hat{B}}|\psi_{\hat{B}}\rangle = \sum_{\delta\gamma}\langle\psi_0|a_\delta^\dagger a_\gamma|\psi_0\rangle\beta_\delta^*(\hat{B})\,\beta_\gamma(\hat{B}) = 1 = \langle\psi_{\hat{A}}|\psi_{\hat{A}}\rangle\,.
$$

If the two-particle density matrix is approximated by an antisymmetrized product of one-particle density matrices one obtains the usual shell-model approximation

$$
{}^1O^{\mathrm{SM}}_{\hat{B}\hat{A}} = \delta_{\hat{B}\hat{A}}\langle\psi_0|{}^1O|\psi_0\rangle - [S(\hat{B})\,S(\hat{A})]^{1/2}\langle\varphi_{\hat{A}}|{}^1O|\varphi_{\hat{B}}\rangle\,,
\tag{7.9}
$$

where $|\varphi_{\hat{B}}\rangle$ and $|\varphi_{\hat{A}}\rangle$ are normalized states defined by

$$
|\varphi_{\hat{B}}\rangle = \frac{|\Phi_{\hat{B}}\rangle}{[S(\hat{B})]^{1/2}}\,.
\tag{7.10}
$$

We stress, however, that, e.g., in the calculation of transition probabilities, the replacement

$$
|\psi_{\hat{B}}\rangle = \sum_\alpha \beta_\alpha a_\alpha|\psi_0\rangle \to \beta_\nu a_\nu|\psi_0\rangle
\tag{7.11}
$$

is not a good approximation because

$$
\beta_\alpha = \langle\Phi_{\hat{B}}|\,D_1^{-1}|\alpha\rangle
$$

and D_1 rapidly decreases for unoccupied states. In fact, our first results show that the coefficients β_ρ are, in general, by no means small compared with β_ν. For this reason the difference between expression (7.8) and the shell-model approximation (7.9) will, in general, be large; it is given by the following expression:

$$
\begin{aligned}
{}^1O_{\hat{B}\hat{A}} - {}^1O^{\mathrm{SM}}_{\hat{B}\hat{A}} = {} & -\langle X_{\hat{A}}|\kappa_2|X_{\hat{B}}\rangle\sum_\alpha\langle\alpha|\kappa_2\,{}^1O|\alpha\rangle + \langle X_{\hat{A}}|\kappa_2\,{}^1O\kappa_2|X_{\hat{B}}\rangle + \sum_{\nu_i\nu_i'}\langle\nu_1\nu_2|\,D_2S_2|\nu_1'\nu_2'\rangle\beta_{\nu_1}(\hat{A})\,\beta_{\nu_1'}^*(\hat{B})\,{}^1O_{\nu_2'\nu_2} \\
& + \sum_{\rho_i\rho_i'}\langle\rho_1\rho_2|S_2D_2|\rho_1'\rho_2'\rangle\beta_{\rho_1}(\hat{A})\,\beta_{\rho_1'}^*(\hat{B})\,{}^1O_{\rho_2'\rho_2} \\
& - 2\sum_{\nu_i\nu_i'\rho_i\rho_i'}\langle\rho_1\rho_2|S_2|\nu_1\nu_2'\rangle\langle\nu_1\nu_2|\,D_2|\rho_1'\rho_2\rangle\,[\beta_{\rho_1}(\hat{A})\,\beta_{\rho_1'}^*(\hat{B})\,{}^1O_{\nu_2'\nu_2} + \beta_{\nu_2}(\hat{A})\beta_{\nu_2'}^*(\hat{B})\,{}^1O_{\rho_1'\rho_1} \\
& \qquad - \beta_{\rho_1}(\hat{A})\beta_{\nu_2'}^*(\hat{B})\,{}^1O_{\rho_1'\nu_2} - \beta_{\nu_2}(\hat{A})\beta_{\rho_1'}^*(\hat{B})\,{}^1O_{\nu_2'\rho_1}] \\
& + \sum_{\rho_i\nu_i}\langle\nu_1\nu_2|D_2|\rho_1\rho_2\rangle\,{}^1O_{\rho_2\nu_2}[\beta_{\nu_1}(\hat{A})\beta_{\rho_1}^*(\hat{B}) + \beta_{\rho_1}(\hat{A})\beta_{\nu_1}^*(\hat{B})]\,,
\end{aligned}
\tag{7.12}
$$

where the operator ${}^1O$ was assumed to be Hermitian and κ_2 is defined by the equation

$$
\kappa_2 = \sum_\nu|\nu\rangle\langle\nu| - D_1
\tag{7.13}
$$

which is a generalization of (4.18a). It is remarkable that the expressions containing the coefficients β_ρ, e.g.,

$$
\sum_{\nu_i\rho_i}\langle\nu_1\nu_2|\,D_2|\rho_1\rho_2\rangle\,{}^1O_{\rho_2\nu_2}\beta_{\nu_1}(\hat{A})\beta_{\rho_1}^*(\hat{B}) = \sum_{\nu_i\rho_i}\langle\nu_1\nu_2|\,D_2|\,\rho_1\rho_2\rangle\,{}^1O_{\rho_2\nu_2}\beta_{\nu_1}(\hat{A})\int\langle\rho_1|\,\vec{r}\rangle\langle\vec{r}\,|D_1^{-1}|\,\vec{r}\,'\rangle\langle\vec{r}\,'|\Phi_{\hat{B}}\rangle d\tau d\tau'\,,
\tag{7.14}
$$

have a behavior resembling the Migdal force, i.e., small in the nuclear interior and strong at the surface.[26]

If the one-hole state is expanded into exact eigenstates of the $(A-1)$-particle system, i.e.,

$$
|\psi_{\hat{B}}\rangle = \sum_i\gamma_i\,|\,\psi_{B_i}\rangle
\tag{7.15}
$$

or

$$
|\Phi_{\hat{B}}\rangle = \sum_i\gamma_i|\Phi_{B_i}\rangle\,,
$$

there arise, in addition to the dominant state, a lot of other states. In this sense it is a matter of taste whether we call our state a "one-hole state" or a "quasihole" state. The term quasihole state might remind the reader of the state-independent effective interaction between quasiparticles and quasiholes shown by Landau[27] for infinite systems. Calling our state a quasihole state does not imply the existence of a similar effective interaction for finite systems as used, without proof, by Migdal.[26]

VIII. CONCLUSION

In this section we start with some concluding remarks on the general relationship between our calculated and experimental energies. Then we discuss whether the empirical shell-model potential can be calculated from *NN* potentials and what conclusions can be drawn from the comparison between our calculated and the experimental energies.

With our methods we may calculate two different quantities, i.e., the centroid energies $\epsilon_{\hat{\beta},\nu}$ and the solutions $\epsilon_{\hat{\beta}}$ (and $|X\rangle$) of (3.7). The state $|\psi_{\hat{\beta}}\rangle$ corresponding to the latter energy is clearly a variational approach to the dominant exact state $|\psi_{\beta}\rangle$, the so-called shell-model state. The energy $\epsilon_{\hat{\beta}}$ and the transition probabilities and expectation values correspondingly are the variational approximations for the *dominant* states. We stress that the energy $\epsilon_{\hat{\beta}}$ should not be compared with an experimental *centroid*, as discussed below.

We would like to make a remark about the relationship of the centroid energy to experiment. Experimentalists cannot investigate centroids of the form (2.5) because the radial dependence of the form factors needed in DWBA calculations is, at least in general, not known. They assume therefore that the form factors may be approximated by shell-model functions multiplied by spectroscopic factors. We believe that this is a reasonable approximation[28,29]; if this were not true it would be very hard to define a reasonable experimental centroid and it would therefore be necessary to calculate the single form factors themselves and then use them in DWBA calculations. In this connection it is very remarkable that our theoretical centroid, given by (3.18), does not strongly depend on $|\alpha\rangle$ provided that "something like a shell-model function" is used for the state $|\alpha\rangle$. In fact, our calculations show that the difference between the "natural-orbital centroid" $\epsilon_{\hat{\beta},\nu}$ and the centroid energy defined by (3.19) is very small, i.e.,

$$|\epsilon_{\hat{\beta},\nu} - \epsilon_{\hat{\beta},\Phi_{\hat{\beta}}}| < 0.03 \text{ MeV}, \tag{8.1}$$

for the p states of ^{15}N and all four potentials we use. This difference would be of the same order if we take an empirical shell-model wave function instead of $|\Phi_{\hat{\beta}}\rangle$ in (3.18). Our theoretical centroids are therefore less state-dependent than the experimental ones. This originates from the fact that C and D are calculated integrating over the whole nucleus whereas both the DWBA and the experimental cross sections mainly depend on the surface parts of the wave functions. Of course, there are centroids which differ appreciably from $\epsilon_{\hat{\beta},\nu}$, e.g., if one takes in (3.18) a state $|\alpha\rangle$ having a wave function which is small in the nuclear interior and large at the surface. The eigenvector $|X\rangle$ of (3.7) is just such a function as may be seen from the Eq. (3.13), i.e.,

$$|X\rangle = D_1^{-1}|\Phi_{\hat{\beta}}\rangle ,$$

and the centroid taken with this function has just the energy $\epsilon_{\hat{\beta}}$; compare (3.17). First results, which we do not give here, show that the difference between $\epsilon_{\hat{\beta}}$ and $\epsilon_{\hat{\beta},\nu}$ is of the order of

$$\epsilon_{\hat{\beta}} - \epsilon_{\hat{\beta},\nu} \approx +2 \text{ MeV}. \tag{8.2}$$

It is, of course, positive because $\epsilon_{\hat{\beta}}$ is the maximum of the theoretical centroids or, more precisely, the maximum of the centroids over all states.

Comparing $\epsilon_{\hat{\beta},\nu}$ (which is the sudden-removal energy of Ref. 4) with experimental centroids we have to consider that experimentalists do not average over all states but only over a part of them. For this reason we approximately eliminated the contribution of the two-hole–one-particle states by solution of (5.3).

Now we discuss the question of whether the shell-model potential can be calculated from the nucleon-nucleon forces. If we are speaking about the shell-model potential we always mean the *empirical* shell model, which describes either the dominant state energies or the centroid energies and the corresponding single-particle (or single-hole) wave functions. Though these potentials are not uniquely defined, the underlying conception is very beautiful and simple and it should be explained by calculations starting from nucleon-nucleon forces without using further parameters. This work is an attempt to do so for one-hole states. There are other, more "theoretical," definitions of the shell model used in order to obtain more rapid convergence in BHF theory.[1,2,30] Our definition is in principle different from those.

We may now define the shell-model potential for the *centroids* of the $(A-1)$-particle states. From the discussion above it is evident that it is sufficient to solve (7.1) in the subspace of occupied states. We have shown in Sec. VII that the operator $C^V D_1^{-1}$ is nearly Hermitian in this subspace if a natural-orbital representation is used. In this sense the operator $C^V D_1^{-1}$ corresponds to an em-

pirical shell-model potential. For the agreement with experiment one should compare Fig. 11.

Usually, the parameters of the empirical shell model are chosen so that they describe the centroids over the weakly excited states rather than the centroids over all states. Therefore the expression

$$C^{V} D_1^{-1} + R(\epsilon_1)$$

should be compared with the empirical shell model where R is a self-energy correction like that given by (5.3) and $|\epsilon_1|$ is somewhat smaller than $|\epsilon_{\hat{B},\nu}|$. In our approach the self-energy correction R is Hermitian; this holds in higher approximations too (Fig. 10).

The shell model may also be defined in such a way that it describes the *dominant* states as one-hole or one-particle states. For one-hole states this corresponds, as we have seen, to the solution of the Eq. (7.1) in the complete Hilbert space of one-particle functions. In this space the operator $C^{V} D_1^{-1}$ is not Hermitian. This means that the form factors of the *dominant* state cannot be described in good approximation by an Hermitian operator. But this is not astonishing: provided that $|\psi_0\rangle$ and $|\psi_B\rangle$ are not pure (antisymmetrized) products of single-particle states, form factors belonging to the same symmetry quantum numbers cannot be *exactly* orthogonal if the corresponding $(A-1)$-particle wave functions are orthogonal. This holds, however, for both sets, the exact states $|\psi_B\rangle$ and our calculated states $|\psi_{\hat{B}}\rangle$. On the other hand, the difference between the energies $\epsilon_{\hat{B}}$ and $\epsilon_{\hat{B},\nu}$ is not very large and the wave functions $\Phi_{\hat{B}}$ are very similar to the single-particle wave functions of the empirical shell models. It will therefore not be difficult to find some empirical shell-model potentials fitting the *calculated* data $\epsilon_{\hat{B}}$ and $\Phi_{\hat{B}}$, at least, if the nucleon-nucleon force from which one starts is not too unrealistic.

From our preliminary results we may conclude something about the two-body potentials we used. One should keep in mind that the results for the 1*s* state cannot be compared directly with experiment for two reasons. The coupling to the p-h excitations of the ^{16}O core is certainly strong and, further, for states in the continuum one needs the spectral function as defined in Ref. 31.

We believe that we have calculated the density matrix and the operator C with sufficiently high accuracy. The uncertainties in the nucleon-nucleon interactions together with corrections of the kind discussed in Sec. V are therefore responsible for the largest part of the uncertainty in the calculations.

As may be seen from Fig. 11 and Tables I and III the HJ potential yields absolute values much too small for both the separation and ground-state energies. Note that the dominant states have an even higher (less negative) energy than the centroids. From the SSCB potential[32] there results a very unrealistic spectrum of ^{39}Ca (Table IV) and a much too high central density in ^{40}Ca and in ^{16}O as shown in Ref. 25. The SSCB potential is therefore also a bad approximation to the *NN* force. The RSC potential yields much better results especially if the three-body correction of Blatt and McKellar is taken into account

The spin-orbit (so) splitting of the BHF energies is nearly the same in GBHF and FBHF(3) calculations. For the final separation energies it is reduced by the "renormalization term" shown in Fig. 9(b) and some three-body correction terms, the most simple of which are shown in Figs. 9(d) and 9(e) and enlarged by the Pauli rearrangement term [Fig. 10(a)].

The final result for the RSC potential is 3.85 MeV and for the $(\mathrm{RSC} + V_{\mathrm{McK}})$ potential, 4.65 MeV. This is much too small if it is compared with the experimental values of 6.32 MeV for the dominant state and 6.87 MeV for the centroids.[18] Since the Pauli rearrangement term [Fig. 10(a)] enlarges the spin-orbit splitting by about 1 MeV in the case of the $(\mathrm{RSC} + V_{\mathrm{McK}})$ potential, one may argue that the influence of the "higher" terms of Fig. 10 is non-negligible. This means that the second term on the right hand side of (2.4) has to be taken into account. On the other hand, Fig. 11 shows that the spin-orbit splitting is very different for various Hamiltonians; 2.6 MeV for the HJ and 6.5 MeV for the SSCB potential, for example. It may therefore be that a relatively large part of the difference of about 2 MeV between the experimental and our theoretical value is due to the uncertainty in the Hamiltonian—especially in view of the approximate nature of the force of Blatt and McKellar.

It was seen that the theory presented in this paper is consistent with basic experimental facts. Therefore we think that it can be regarded as the lowest-order approximation. We suggest that in treating higher orders the contribution of excited core states should be taken into account.

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APPENDIX A

The single-particle Green's function is defined by

$$g(\vec{r}t,\vec{r}'t') = \frac{1}{i}\langle\psi_0|\mathcal{T}a(\vec{r},t)a^\dagger(\vec{r}',t')|\psi_0\rangle$$
$$= g(\vec{r},\vec{r}',t-t'), \tag{A1}$$
$$a(\vec{r},t) = e^{iHt}a(\vec{r})e^{-iHt},$$
$$a(\vec{r}) = \sum_\alpha a_\alpha\langle\vec{r}|\alpha\rangle,$$

where $\mathcal{T}$ is the time ordering operator. The Fourier transform is given by

$$g(\vec{r},\vec{r}',\omega) = \int_{-\infty}^{\infty} d\tau\, g(\vec{r},\vec{r}',\tau)e^{i\omega\tau}$$
$$= \sum_{B(A+1)} \frac{\langle\psi_0|a(\vec{r})|\psi_B\rangle\langle\psi_B|a^\dagger(\vec{r}')|\psi_0\rangle}{\omega-[E_B(A+1)-E_0(A)]+i\delta}$$
$$+ \sum_{B(A-1)} \frac{\langle\psi_0|a^\dagger(\vec{r}')|\psi_B\rangle\langle\psi_B|a(\vec{r})|\psi_0\rangle}{\omega-[E_0(A)-E_B(A-1)]-i\delta}. \tag{A2}$$

Using (2.1) this reads

$$g(\vec{r},\vec{r}',\omega) = \sum_{B(A+1)} \frac{\Phi_B(\vec{r})\Phi_B^*(\vec{r}')}{\omega-[E_B(A+1)-E_0(A)]+i\delta}$$
$$+ \sum_{B(A-1)} \frac{\Phi_B(\vec{r})\Phi_B^*(\vec{r}')}{\omega-[E_0(A)-E_B(A-1)]-i\delta}. \tag{A3}$$

The functions $\Phi_B(\vec{r})$ evidently diagonalize the Green's function at the poles. The right hand side of (A3) is, however, not a spectral representation of g because the form factors are in general, not orthogonal. The operators C and D are related to the Green's function by the equations

$$C = \lim_{\tau\to-0}\frac{\partial g}{\partial t}\bigg|_{t=\tau} \tag{A4}$$

$$D = \frac{1}{i}\lim_{\tau\to-0} g(\tau). \tag{A5}$$

APPENDIX B

We remark that both operators D and C are compact. Because they are positive and negative, respectively, we have, following, e.g., theorem 42 of Chap. 5 of Ref. 33, only to show that the traces of these operators are bounded. This is evident because from (3.9) and (3.6) there follows

$$\sum_\alpha C_{\alpha\alpha} = \langle\psi_0|T|\psi_0\rangle + 2\langle\psi_0|V|\psi_0\rangle$$
$$= 2E_0 - \langle\psi_0|T|\psi_0\rangle, \tag{B1}$$

$$\sum_\alpha D_{\alpha\alpha} = A. \tag{B2}$$

In its diagonal representation (natural-orbital representation) the operator D may be written in the following way

$$D = \begin{pmatrix} \rho_1 & 0 & 0 & \cdots \\ 0 & \rho_2 & 0 & \cdots \\ 0 & 0 & \rho_3 & \cdots \\ \vdots & & & \end{pmatrix}, \quad \rho_1 \geq \rho_2 \geq \rho_3 \geq \cdots, \tag{B3}$$

where the multiplicity of every eigenvalue is finite. The positive compact operator $-C$ may be written in a similar way.

To prove the assertion made after Eq. (3.14) we assume

$$\langle\psi_{\hat{B}}|\psi_{\hat{B}}\rangle = \frac{\langle X|D|X\rangle}{\langle X|X\rangle} = d > 0. \tag{B4}$$

Because the operator D is compact there is a finite dimensional operator $D^{(N)}$ so that

$$D = D^{(N)} + \tilde{D} \tag{B5}$$

with

$$||\tilde{D}|| \leq \delta, \tag{B6}$$

where δ is an arbitrarily small positive number if N is large enough. The compact operator C may be analogously decomposed. If we let

$$\frac{\langle X|\tilde{D}|X\rangle}{\langle X|X\rangle} = \eta, \quad 0 \leq \eta \leq \delta, \tag{B7}$$

it follows that

$$\epsilon_{\hat{B}} = \frac{\langle X|C|X\rangle}{\langle X|D|X\rangle} = \frac{\langle X|C^N|X\rangle}{\langle X|D^N|X\rangle[1+\eta/(d-\eta)]} + \frac{\langle X|\tilde{C}|X\rangle}{d}$$
$$= \frac{\langle X|C^N|X\rangle}{\langle X|D^N|X\rangle} + \lambda, \tag{B8}$$

where, for large N, λ can be neglected compared with the first term. Note that the absolute value of this quotient cannot be small because the inequality (3.12) holds.

The wave function $|\Phi_{\hat{B}}\rangle$ is given by

$$|\Phi_{\hat{B}}\rangle = D|X\rangle = \sum_{\alpha\leq N} D|\alpha\rangle\langle\alpha|X\rangle + \sum_{\alpha>N} D|\alpha\rangle\langle\alpha|X\rangle. \tag{B9}$$

For large N the second term is negligible; the convergence is especially rapid if one uses the set of natural orbitals for $\{|\alpha\rangle\}$. We have still to prove that equations

$$\langle\psi_{\hat{B}}|\psi_{\hat{B}}\rangle = \frac{\sum_n \langle X|n\rangle\rho_n\langle n|X\rangle}{\langle X|X\rangle} = 0, \tag{B10}$$

$|n\rangle$ = natural orbital

and

$$S(\hat{B}) = \frac{\langle X|D^{+}D|X\rangle}{\langle X|D|X\rangle} = 0 \tag{B11}$$

are equivalent. From (B10) it follows that

$$\langle n|X\rangle = 0 \tag{B12}$$

for all n because D is positive. From this it follows that

$$D|X\rangle = 0, \tag{B13}$$

and therefore (B11) holds. Vice versa, from (B11) follows the equations (B13) and therewith (B10).

APPENDIX C: CENTER-OF-MASS CORRECTIONS

Though the energies h_ν contain the usual A-particle c.m. corrections, there arise additional correction terms if separation energies are calculated.[34] We start from the exact equation

$$\langle\psi_B|H_{\text{int}}a_\alpha|\psi_0\rangle - \langle\psi_B|a_\alpha H_{\text{int}}|\psi_0\rangle = [E_B(A-1) - E_0(A)]\langle\psi_B|a_\alpha|\psi_0\rangle \tag{C1}$$

with

$$\langle\psi'_A|H_{\text{int}}|\psi_A\rangle = \left\langle\psi'_A\middle|\frac{1}{2}\sum_{i\neq j}V_{ij} + \left(1-\frac{1}{A}\right)\sum_{i=1}\frac{p_i^2}{2m} - \frac{1}{A}\sum_{i\neq j}\frac{\vec{p}_i\vec{p}_j}{2m}\middle|\psi_A\right\rangle, \tag{C2}$$

where $|\psi_A\rangle$ and $|\psi'_A\rangle$ are eigenstates of the particle number operator. We obtain from (C1) and (C2)

$$\left\langle\psi_B\middle|\left\{\left[\left(1-\frac{1}{A}\right)T - \frac{1}{A}T_{\text{II}} + V\right]_1 a_\alpha\right\}\middle|\psi_0\right\rangle - \frac{1}{A(A-1)}\langle\psi_B|(T+T_{\text{II}})a_\alpha|\psi_0\rangle = -\epsilon_B\langle\psi_B|a_\alpha|\psi_0\rangle, \tag{C3}$$

where

$$T_{\text{II}} = \sum_{i\neq j}\frac{\vec{p}_i\vec{p}_j}{2m}, \quad T = \sum_i\frac{p_i^2}{2m}.$$

We replace the exact solution $|\psi_B\rangle$ by the ansatz (3.1). The term $(T+T_{\text{II}})/A$ in the commutator is already contained in C so that we obtain, instead of (3.7), the corrected equation

$$\sum_{\alpha'}\left[C_{\alpha\alpha'} + \frac{1}{A(A-1)}\left(\sum_{\gamma_1\gamma_2}\langle\gamma_1|T|\gamma_2\rangle\langle\alpha\gamma_2|D_2|\alpha'\gamma_1\rangle\right)\right.$$
$$\left. + \frac{1}{2}\sum_{\gamma_i}\langle\gamma_1\gamma_2|T_{\text{II}}|\gamma_3\gamma_4\rangle\langle\alpha\gamma_3\gamma_4|D_3|\alpha'\gamma_1\gamma_2\rangle - \epsilon_{\hat{B}}\langle\alpha|D_1|\alpha'\rangle\right]\beta^*_{\alpha'} = 0. \tag{C4}$$

The correction term containing the operator T is in first approximation given by the expression

$$\frac{1}{A(A-1)}\sum_{\nu\nu'}\delta_{\nu\alpha}\delta_{\nu'\alpha'}\left(\delta_{\nu\nu'}\sum_\mu\langle\mu|T|\mu\rangle - \langle\nu|T|\nu'\rangle\right). \tag{C5}$$

It is evidently of the order $A^{-1}T$. The corresponding correction for the energy $\epsilon_{\hat{B},\nu}$, given by (4.21), reads

$$\frac{1}{A(A-1)}\;\frac{1}{1-\langle\nu|\chi_2|\nu\rangle}\sum_{\mu\neq\nu}\langle\mu|T|\mu\rangle. \tag{C6}$$

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*Present address: Institut für Theoretische Physik der Ruhruniversität Bochum, W- t Germany.
†Present address: Laboratory for Nuclear Science and Department of Physics, MIT, Cambridge, Massachusetts 02139.
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[12]From (3.14) there follow the inequalities

$$\rho_n^{\max}(j,\pi,m) \geq S(\hat{B}) \geq \langle X|D|X\rangle / \langle X|X\rangle .$$

Note also that the relations

$$1 > \sum_B{}^{*} \langle \Phi_B|\Phi_B\rangle = \sum_n{}^{*} \rho_n > \rho_n^{\max}(j,\pi,m)$$

($\sum_B{}^{*}$ and $\sum_n{}^{*}$ mean: j, π, m given) hold where ρ_n are the eigenvalues of D; compare the Appendix B.

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