Multiconfigurational Self-Consistent Calculation in Light Deformed Nuclei*

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A variational method of calculating correlated intrinsic wave functions for deformed nuclei is formulated. The configuration amplitudes and the single-particle orbitals which define such wave functions obey a system of equations, which is solved self-consistently by an iterative procedure for the doubly even $N=Z$ nuclei in the *sd* shell. The correlations under study are of the 2p-2h type. Compared with the independent-particle Hartree-Fock picture, the present solutions show a greater stability in terms of binding energy and shape symmetry.

I. INTRODUCTION

In many fields of physics most of the many-particle systems can be described approximately, but often very successfully, by means of a simple model known under different names but based on the same basic idea that each particle moves independently of all others in a common field which depends on the average motion of all particles involved. The total wave function is then a simple product, properly symmetrized or antisymmetrized, of the individual particle wave functions. In particular, in the study of deformed atomic nuclei such wave functions are customarily taken as the eigenstates of a nonspherical potential parametrized to fit experimental data,[1] or to minimize the total energy.[2,3] Or they can be obtained in a more fundamental manner from the nuclear Hamiltonian along the well-known Hartree-Fock (HF) variational scheme.[4,5]

Many HF calculations have been performed and have been brought to bear on the observed nuclear properties.[6] Because of their apparently deformed shapes, because of their simple symmetries, and finally because of the wealth of experimental data available, the doubly even $N=Z$ nuclei in the *sd* shell have been most extensively studied. Perhaps the most significant result of these calculations is the existence of an energy gap between the occupied and unoccupied single-particle levels. This single-particle energy gap determines the degree of stability of the HF configuration against particle excitations, and hence the extent to which the independent-particle picture is valid. In the first half of the *sd* shell and more particularly in the ^{20}Ne nucleus, the single-particle gap is large for the most stable solution, and the HF scheme has known considerable success.

Unfortunately, for many nuclei, the variational HF procedure yields several solutions, most of which do not exhibit a large single-particle energy gap. If these solutions are degenerate or nearly degenerate, as is often the case, the minimal-energy criterion alone can no longer be relied upon to choose the correct solution, since the energy fluctuation and the second-order potential energy may both be appreciable. Moreover, in the past few years, several experimental groups[7,8] using techniques of heavy-ion Coulomb excitation, particle transfer, and inelastic reactions have collected new data, many of which challenge the predictions of the HF method. These difficulties, not to mention the complete failure of the HF method in the second half of the *sd* shell, clearly point out the limitations of the independent-particle picture, and indicate the necessity of including the correlation between the individual motions in the intrinsic wave function. In this connection pairing correlations immediately come to mind. The importance of pairing phenomena in heavy nuclei has long been recognized; and a proper formalism treating the pairing correlations and the underlying field on the same basis has been known for some time under the name of the Hartree-Fock-Bogoliubov (HFB) method.[9,10] Recently it has been applied in all its generality in a numerical study of light deformed nuclei.[11,12] The results show that while the $T=1$ pairing is almost nonexistent, the $T=0$ pairing affects the nuclear structure in many important ways, such as by restoring the shape symmetry in several nuclei.

The HFB method deals with a special class of correlations. This paper investigates a more general method of obtaining correlated intrinsic wave functions. Dubbed the multiconfigurational self-consistent (MCSC) field theory, it has been known and used for some time in atomic and molecular physics.[13] It consists of assuming the total wave function to be a superposition of elementary states representing specific particle correlations, and of obtaining the particle orbitals and the configuration-mixing coefficients in a completely self-consistent manner. Although for obvious reasons some restriction must be placed upon the number

of configurations actually calculated, there are in principle no limitations on their nature or their relative importance. That this approach is also practical and useful in nuclear physics has been demonstrated by the recent calculations of Satpathy and Ho-Kim[14] and Faessler, Plastino, and Schmid.[15]

In the following section details on the MCSC method will be presented. The problem of minimizing the energy of a many-body assembly reduces to solving a system of coupled equations which the particle orbitals and the configuration amplitudes satisfy. It will be shown that the MCSC field has the same formal structure as the HF field, and can be represented in terms of one-body and two-body density matrices. In Sec. III we use the even-even $N=Z$ nuclei in the *sd* shell to illustrate the practical aspect of the method. In particular, the choice of configurations and a computational scheme will be discussed at length. Although the set of configurations actually included in our calculations might be too restricted to describe accurately the real physical situation, the results nevertheless already exhibit many interesting effects. Finally, a theory recently advanced by Padjen and Ripka,[16] also aimed at obtaining the correlation energy, will be discussed and compared with the present method. Section IV contains our conclusions.

II. MCSC METHOD

The MCSC method develops a variational procedure by which the wave function of an N-particle system can be determined. Let us first introduce a certain orthonormal complete set of one-particle wave functions, or orbitals, ordered so that the first M ($M \geq N$) orbitals may be occupied; all others remain unoccupied. The trial wave function of the system Ψ is then chosen to be a linear combination of antisymmetrized normalized products Φ_I of N orbitals selected from the set of the first M orbitals:

$$|\Psi\rangle = \sum_I |\Phi_I\rangle\langle\Phi_I|\Psi\rangle = \sum_I |\Phi_I\rangle C_I . \tag{1}$$

There are $\binom{M}{N}$ such determinantal functions Φ_I; each represents a configuration of occupied orbitals. In particular, we call Φ_0, or Φ_{HF}, the reference (0p-0h) configuration, in which the lowest N single-particle states are filled.

Let the total Hamiltonian of the system have the standard second-quantized form:

$$H = \sum \langle\alpha|t|\beta\rangle a_\alpha^\dagger a_\beta + \tfrac{1}{4}\sum \langle\alpha\beta|V|\gamma\delta\rangle a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma , \tag{2}$$

where the two-body matrix element is antisymmetrized. The expectation value of H in the state Ψ may be expressed in two equivalent forms:

$$\langle H\rangle = \sum_{I,I'} C_I^* \langle\Phi_I|H|\Phi_{I'}\rangle C_{I'} \tag{3a}$$

$$= \sum_{\lambda=1}^{M} (\langle\lambda|t\gamma|\lambda\rangle + \tfrac{1}{2}\sum_\mu \langle\lambda\mu|V\Gamma|\lambda\mu\rangle) , \tag{3b}$$

where here and throughout this paper the indices $\lambda, \mu, \ldots$ denote occupied single-particle states. In the last equation the one-body and two-body density operators have been introduced and are defined by:

$$\langle\beta|\gamma|\alpha\rangle = \langle a_\alpha^\dagger a_\beta\rangle , \tag{4}$$

$$\langle\gamma\delta|\Gamma|\alpha\beta\rangle = \tfrac{1}{2}\langle a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma\rangle . \tag{5}$$

They are Hermitian and are normalized by their traces: $\mathrm{Tr}\gamma = N$ and $\mathrm{Tr}\Gamma = \frac{1}{2}N(N-1)$. In general the one-body density is not diagonal, though it is useful to find a representation in which it is, in which case its diagonal matrix elements may be interpreted as the occupation numbers of occupied orbits. The two-body density describes particle correlations, the nature of which depends on the configurations chosen; in fact its matrix elements give complete knowledge of any system governed by a force of the type (2).

The variational principle states that the energy of the ground state is the lower bound of $\langle H\rangle$ for any arbitrary normalized trial wave function, and further that all eigenstates of the system obey the condition

$$\delta\langle H\rangle = 0 \tag{6}$$

under arbitrary infinitesimal changes in the trial wave function, subject to the orthonormality constraint of the eigenstates and the particle orbitals. Independent variations of the configurations and orbitals lead to a system of coupled equations:

$$\sum_{I'} (\langle\Phi_I|H|\Phi_{I'}\rangle - E\delta_{II'}) C_{I'} = 0 , \tag{7a}$$

$$\langle\lambda|t\gamma|\mu\rangle + \sum_{\nu=1}^{M} \langle\lambda\nu|V\Gamma|\mu\nu\rangle - \epsilon_{\lambda\mu} = 0 . \tag{7b}$$

The Lagrangian multiplier E assumes the usual meaning of the energy of the system in some state Ψ_n. The Lagrangian multiplier matrix ϵ, introduced to preserve the orthonormality of the orbitals, is Hermitian, $\epsilon_{\lambda\mu} = \epsilon_{\mu\lambda}^*$, and in general non-diagonal.

If the coefficients C_I are not explicit functions of the orbitals, the infinitesimal variations leading to Eq. (7b) can be generated by a unitary transformation $\exp\sum(z_{\alpha\beta}a_\alpha^\dagger a_\beta - z_{\alpha\beta}^* a_\beta^\dagger a_\alpha)$, defined in terms of the arbitrary infinitesimal complex quantities $z_{\alpha\beta}$. The variational condition (6) then becomes

$$\langle[H, \sum(z_{\alpha\beta}a_\alpha^\dagger a_\beta - z_{\alpha\beta}^* a_\beta^\dagger a_\alpha)]\rangle = 0 , \tag{8}$$

or, since both the real and imaginary parts of z are arbitrary, more simply:

$$\langle [a_\alpha^\dagger a_\beta, H] \rangle = 0 . \tag{9}$$

If $\alpha = \lambda$, an occupied state, and $\beta = \eta$, an unoccupied state, we obtain

$$\langle \Psi | a_\lambda^\dagger a_\eta H | \Psi \rangle = 0 . \tag{10}$$

This relation expresses the fact that the Ψ resulting from an energy minimization of the type (8) is not directly coupled by H to singly excited states, $a_\eta^\dagger a_\lambda | \Psi \rangle$; i.e., those formed by promoting a particle from the space of occupied orbits into the complementary space.

In the standard HF method, a possible form of the energy-minimization condition is

$$\langle \alpha_0 | [h_0, \gamma_0] | \beta_0 \rangle = 0 , \tag{11}$$

where all quantities refer to the HF approximation, and h_0 stands for the self-consistent field. From this equation follows a particularly useful result: $\langle \eta_0 | h_0 | \lambda_0 \rangle = 0$, which says that the occupied subspace λ_0 is completely separated from the empty subspace η_0. These relations have their counterparts in the MCSC method. Let us substitute the Hamiltonian (2) into Eq. (9) and recall the definition of the density operators; we then obtain for any orbitals α, β:

$$\langle \alpha | [t, \gamma] + \mathrm{Tr}_2 [V_{12}, \Gamma_{12}] | \beta \rangle = 0 , \tag{12}$$

where it is understood that the trace Tr_2 operates on the variables of the second particle. The last equation contains the one- and two-body operators of the Hamiltonian instead of a self-consistent-field operator as in Eq. (11). Nevertheless, it is helpful to introduce here an MCSC field operator, which we define by

$$h = \sum_{\alpha\beta} (\langle \alpha | t \gamma | \beta \rangle + \sum_\delta \langle \alpha\delta | V \Gamma | \beta\delta \rangle) a_\alpha^\dagger a_\beta . \tag{13}$$

It correctly reduces to the HF field h_0 in the limiting case $M = N$. It is Hermitian and, furthermore, has vanishing matrix elements between occupied and unoccupied states if the densities γ and Γ through which it is defined are calculated with the right wave function Ψ; i.e., that for which the energy is stationary with respect to variations in the orbitals.

Thus two important properties of the HF theory, expressed in Eqs. (10) and (11), still stand in the MCSC theory, but in modified and weakened forms. In particular, while the HF condition $\langle \eta_0 | h_0 | \lambda_0 \rangle = 0$ suggests a diagonalization of h_0, which then yields the orbitals, a diagonalization of the MCSC field h offers no great advantage because in the present case the entire single-particle space ($\lambda \leq M$) is used to construct the determinants; the occupied state η in $\langle \eta | h | \lambda \rangle = 0$ stays completely outside the space under consideration ($\eta > M$). Thus one may as well solve Eq. (7b) directly for the occupied orbitals $| \lambda \rangle$.

III. APPLICATION TO *sd* SHELL NUCLEI

The MCSC method is in principle quite simple. Its basic content is summarized in Eqs. (7), which we now proceed to solve. Two difficulties become immediately apparent: the size of the system of equations to be solved, and their nonlinear nature. We devise a practical iterative scheme of solution and apply it to a study of the intrinsic structure of the ground states of even-even $N = Z$ nuclei in the *sd* shell.

A. Choice of Configurations

The size of the MCSC system of equations depends on both the single-particle space and the configurations used in the construction of the trial wave function. Following a well-established custom of workers in the field, we consider ^{16}O as an inert core and define our active single-particle space as that spanned by the entire *sd* shell.

Even in this modest space the number of possible configurations is beyond our practical computational means. It can, however, be reduced further by taking into account symmetry laws. The HF configuration Φ_0 is probably, but not necessarily, the dominant one. For the nuclei under consideration we may assume it to be symmetric under the exchange of protons and neutrons, to have zero isospin, and, moreover, to be time-reversal-invariant. We also assume axial symmetry. Each orbital is then characterized by a quantum number k, an eigenvalue of the angular momentum component j_z; the wave function Φ_0 is an eigenstate of the total angular momentum component J_z of eigenvalue $K = 0$. Then with the nuclear Hamiltonian usually assumed, the excited configurations Φ_I must be chosen to have the same symmetry properties as Φ_0.

Since the lowest-order perturbative correction to the HF energy comes from the 2p-2h excitations of Φ_0, we assume that the ground-state correlations are mainly produced by such states. We shall denote each orbital by $\alpha = (a, t_a)$, where the Latin symbol stands for all quantum numbers except the charge t_a. Then a 2p-2h configuration of total isospin zero can be formed from a pair of particles ($\nu\nu'$) and a pair of holes ($\lambda\lambda'$), each coupled to isospin T_0:

$$| nn' ll' (T_0) \rangle = (2T_0 + 1)^{-1/2} \sum_{M_0} A^\dagger (nn' T_0 M_0) \times A(ll' T_0 M_0) | \Phi_0 \rangle , \tag{14}$$

where it is observed that $\langle T_0 M_0 T_0 -M_0 | 00\rangle = (-)^{T_0-M_0}(2T_0+1)^{-1/2}$, and where the following notation is used:

$$A^\dagger(abTM) = \epsilon(ab)\sum_{t_a t_b}\langle \tfrac{1}{2}t_a \tfrac{1}{2}t_b | TM\rangle a^\dagger_\alpha a^\dagger_\beta ,$$

$$\epsilon(ab) = 1 \qquad a \neq b$$
$$= 1/\sqrt{2} \qquad a = b, \quad T = 0$$
$$= 0 \qquad a = b, \quad T = 1 .$$

If a configuration contains time-reversed pairs, that is, if $n' = \tilde{n}$ and $l' = \tilde{l}$, it is taken as in Eq. (14); otherwise a time-reversal-invariant state is formed by the combination

$$\sqrt{\tfrac{1}{2}}\,[\,|nn'll'(T_0)\rangle + |\tilde{n}\tilde{n}'\tilde{l}\tilde{l}'(T_0)\rangle\,] .$$

Finally we introduce the requirement that no two configurations be connected through single-particle excitations. The only reason for this arbitrary restriction is that it makes the one-body density operator diagonal, and that it reduces the number of configurations. The configurations actually included in the present calculations are illustrated in Fig. 1; there are 13, 18, 22, 20, and 13 of them for ^{20}Ne, ^{24}Mg, ^{28}Si, ^{32}S, and ^{36}Ar, respectively.

In mixing deformed configurations in the intrinsic state, care should be taken to avoid the spurious effects which result from nonconservation of angular momentum. These arise, for example, from a rotation of the 0p-0h wave function; such a rotated state clearly overlaps with other components of the total wave function and produces extraneous energy gains which must not be confused with the energy gains from particle correlations.

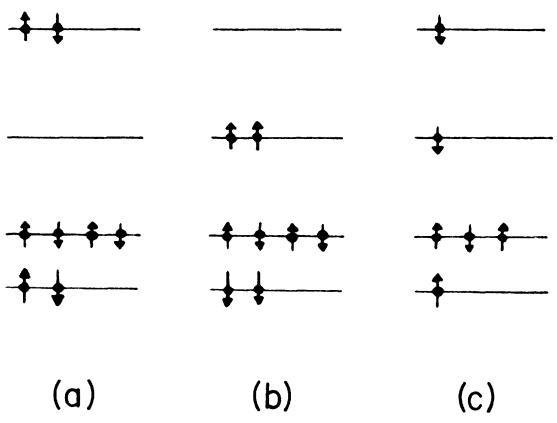

FIG. 1. 2p-2h configurations. Included in the present calculations are: (a) configurations formed by time-reversed pairs of isospin $T_0 = 0$, 1; and (b) configurations formed by nonidentical-particle pairs of $T_0 = 0$. The more general 2p-2h configurations of type (c) are not included.

We meet this difficulty by explicitly constructing and eliminating the state $J^2|\Phi_0\rangle$, which is the main component of the rotated state of Φ_0 on the 2p-2h configurations. Other possible spurious admixtures, such as $J^4|\Phi_0\rangle$, are ignored. The validity of this approximate treatment has been discussed in Ref. 16. When components such as $J^2|\Phi_0\rangle$ are removed the coefficients C_I for $I \neq 0$ become dependent in effect on $|\Phi_0\rangle$ and hence on the orbitals which go into it. Then Eqs. (7) and (12) are not quite valid. If C_I for $I \neq 0$ are small compared with C_0, the error introduced will be correspondingly small, which we assume.

B. Numerical Procedure

Calculations are performed in a shell-model basis. The orbitals are expanded in terms of the eigenstates $2s_{1/2}$, $1d_{3/2}$, and $1d_{5/2}$ of a spherical harmonic oscillator:

$$|\lambda\rangle = \sum_j |jm\rangle c^\lambda_{jm} , \tag{15}$$

where $m = k_\lambda$ to conform to axial symmetry. We use the Condon-Shortley phase convention; it follows from the assumed time-reversal and parity invariance that the coefficients c are real. We keep $1s$ and $1p$ shells closed, and parametrize the single-particle operator of the Hamiltonian in the form

$$e_j = e_0 + \alpha_{ls}\langle j\,|\vec{l}\cdot\vec{s}\,|j\rangle + \alpha_{l^2}\vec{l}^2 . \tag{16}$$

Two sets of parameters will be used: The first is identical to the one used in Ref. 5, with $e_0 = -4.2$, $\alpha_{ls} = -2.8$, and $\alpha_{l^2} = 0$ MeV; the second fits experimental single-particle energies (in the ^{28}Si region), with $e_0 = -3.88$, $\alpha_{ls} = -2.12$, and $\alpha_{l^2} = 0.12$ MeV. The two-body potential is taken to be the Yale potential.[17] This potential has been determined by an accurate fitting to the nucleon-nucleon scattering data. Since it has a hard core, it is to be replaced by a nonsingular reaction matrix. We use the reaction matrix elements for the oscillator parameter $b = (\hbar/m\omega)^{1/2} = 1.76$ F, calculated and tabulated by Shakin, Waghmare, and Hull.[18]

We propose to solve the system of Eqs. (7) by iteration. Once the matrix elements of the Hamiltonian H are known, Eq. (7a) is a secular equation in C_I and can easily be dealt with. In contrast, Eq. (7b) is nonlinear in the unknown c_i, and some calculational scheme has to be devised. Adopting a technique of the HF method, we seek to linearize our MCSC equation. One way to do it is to use the shell-model expansion (15) and rewrite Eq. (7b) as follows:

$$\sum_{j'}\langle j|h|j'\rangle c^\mu_{j'} = \sum_\lambda \epsilon_{\lambda\mu} c^\lambda_j , \tag{17}$$

where

$$\langle j|h|j'\rangle=\langle j|t\gamma|j'\rangle+\sum_{\nu}\langle j\nu|V\Gamma|j'\nu\rangle. \tag{18}$$

Assuming $\langle j|h|j'\rangle$ and $\epsilon_{\lambda\mu}$ are known from previously calculated values of C_I and c_i, one can consider the above equation as linear in c and seek its solutions accordingly. However, when the energy operators are expressed in the shell-model representation and the density operators in the orbital representation, as is necessary for computational purposes, the matrix elements $\langle j|h|j'\rangle$ depend on a product of 4 c's. Consequently, an iterative scheme based on Eq. (17) is bound to be at best slowly convergent.

Another possible approach starts with the observation that Γ can be split into two parts: $\Gamma=P+\Delta$, where P is diagonal and Δ nondiagonal in the space of the configurations, and that the two parts are not equally important in the buildup of the binding energy. The situation is fairly clear if isospin coupling is ignored, and it will temporarily be so assumed. The matrix elements of P will then exhibit the following structure:

$$\begin{aligned}\langle\delta\gamma|P|\alpha\beta\rangle&=\sum_I C_I{}^2\langle\Phi_I|\tfrac{1}{2}a_\alpha^\dagger a_\beta^\dagger a_\gamma a_\delta|\Phi_I\rangle,\\&=\tfrac{1}{2}(\delta_{\alpha\delta}\delta_{\beta\gamma}-\delta_{\alpha\gamma}\delta_{\beta\delta})\sum_I C_I{}^2\rho_\alpha(I)\rho_\beta(I),\end{aligned} \tag{19}$$

with

$$\rho_\alpha(I)=\langle\Phi_I|a_\alpha^\dagger a_\alpha|\Phi_I\rangle.$$

This shows that P contains statistical correlations of the system. Dynamical correlations are in Δ. Consider then the equation

$$\sum_{\mu' i'}(\langle i|t|i'\rangle\gamma_{\mu'\mu}+\sum_{jj'}\langle ij|V|i'j'\rangle\langle\mu'j'|P|\mu j\rangle)c_{i'}^{\mu'}=\sum_\lambda\epsilon_{\lambda\mu}c_i^\lambda-W_i^\mu, \tag{20}$$

where

$$W_i^\mu=\sum_\nu\langle i\nu|V\Delta|\mu\nu\rangle,$$

$$\langle\mu'j'|P|\mu j\rangle=\sum_{\nu\nu'}\langle\mu'\nu'|P|\mu\nu\rangle c_j^\nu c_{j'}^{\nu'},$$

and observe that it reduces to an even simpler form if γ is diagonal in the orbital representation and if isospin coupling is again ignored:

$$\sum_{i'}(\langle i|t|i'\rangle\gamma_\mu+\langle i|U_\mu|i'\rangle)c_{i'}^\mu=\sum_\lambda\epsilon_{\lambda\mu}c_i^\lambda-W_i^\mu, \tag{21}$$

where

$$\langle i|U_\mu|i'\rangle=\sum_{jj'}\langle ij|V|i'j'\rangle\sum_\nu c_j^\nu c_{j'}^\nu\sum_I C_I{}^2\rho_\mu(I)\rho_\nu(I).$$

The main advantage of this equation over Eq. (17) is that the "large" contribution, given by the expression in parentheses on the left-hand side, depends only quadratically on the coefficient c_i. Use of the correct wave functions (14) would leave the form of Eq. (21) unchanged, although of course P and hence U_μ would contain sums over isospin quantum numbers, which can, however, be reduced by invoking charge symmetry. Finally, to transform the above relation into a vector equation for a given $|\mu\rangle$, and further to ensure the requirement $\epsilon_{\lambda\mu}=\epsilon_{\mu\lambda}^*=\epsilon_{\mu\lambda}$, we replace $\epsilon_{\lambda\mu}$ for $\lambda\neq\mu$ by

$$\hat{\epsilon}_{\lambda\mu}=\tfrac{1}{2}(\epsilon_{\lambda\mu}+\epsilon_{\mu\lambda}). \tag{22}$$

Using Eq. (21), along with the orthonormality of the vectors $|\mu\rangle$, we calculate $\epsilon_{\lambda\mu}$, then $\hat{\epsilon}_{\lambda\mu}$, which is fed back into (21) to give

$$\sum_{i'}\langle i|M_\mu|i'\rangle c_{i'}^\mu=-\hat{W}_i^\mu, \tag{23}$$

where

$$M_\mu=\hat{t}_\mu+\hat{U}_\mu-\epsilon_\mu; \tag{24}$$

$$\langle i|\hat{t}_\mu|i'\rangle=\langle i|t|i'\rangle\gamma_\mu-\tfrac{1}{2}\sum_j\sum_{\lambda\neq\mu}\langle j|t|i'\rangle(\gamma_\mu+\gamma_\lambda)c_i^\lambda c_j^\lambda, \tag{25a}$$

$$\langle i|\hat{U}_\mu|i'\rangle=\langle i|U_\mu|i'\rangle-\tfrac{1}{2}\sum_j\sum_{\lambda\neq\mu}\langle j|U_\mu+U_\lambda|i'\rangle c_i^\lambda c_j^\lambda, \tag{25b}$$

$$\hat{W}_i^\mu=W_i^\mu-\tfrac{1}{2}\sum_j\sum_{\lambda\neq\mu}(W_j^\mu c_j^\lambda+W_j^\lambda c_j^\mu)c_i^\lambda, \tag{25c}$$

$$\epsilon_\mu=\sum_{ii'}\langle i|t\gamma_\mu+U_\mu|i'\rangle c_i^\mu c_i^\mu+\sum_i W_i^\mu c_i^\mu. \tag{25d}$$

Thus the equation to be solved for c_i is nonhomogeneous, $\hat{W}\neq 0$, and its resolvent operator M_μ depends on the vector $|\mu\rangle$ to be found.

In summary, our computational scheme is based on Eqs. (7a) and (23)–(25). The starting solutions are taken to be the HF (or Nilsson-type) orbitals having appropriate symmetry properties, together with the coefficients $C_0=1$ and $C_I=0$ for $I\neq 0$. Each iterative cycle includes the following successive steps:

(i) The matrix elements of H are calculated in the configuration space purified of its spurious components, and Eq. (7a) is solved by diagonalization. The solution of lowest eigen energy gives the ground-state vector $\{C_I\}$.

(ii) For each orbital $|\mu\rangle$ the matrix elements $\langle i|M_\mu|i'\rangle$ and the vector components $\hat{W}_i^\mu$ are calculated using the definitions (24) and (25), together with the presently available values of C_I and c_i.

(iii) The components c_i^μ of each vector $|\mu\rangle$ are found from the linear equation (23) by inverting the matrix M_μ.

(iv) All vectors $|\mu\rangle$ thus obtained are normalized and orthogonalized by the Schmidt method.

TABLE I. Orbit wave functions for the lowest axially symmetric deformed solutions in the even-even $N=Z$ nuclei in the *sd* shell. For each entry the upper line refers to the HF approximation, the lower to the MCSC approximation. For each nucleus, the particle strengths in the spherical-basis states are first given, then the occupation density γ_k and the single-particle vector components c_{jk} are shown. Finally we list the binding energy (in MeV), the quadrupole and hexadecapole moments Q_2 and Q_4 (in units of b = 1.76 F), and the 0p-0h probability. The single-particle energies used for ^{28}Si are: $e_{s_{1/2}}=-3.88$, $e_{d_{3/2}}=0.0$, $e_{d_{5/2}}=-5.30$ MeV; and for other nuclei: $e_{s_{1/2}}=-4.20$, $e_{d_{3/2}}=0.0$, $e_{d_{5/2}}=-7.0$ MeV.

k	γ_k	$s^k_{1/2}$	$d^k_{3/2}$	$d^k_{5/2}$
		^{20}Ne		
		0.1564	0.1192	0.7244
		0.1536	0.1203	0.7260
$\frac{1}{2}$	1.0000	−0.3955	−0.3453	0.8511
	0.9949	−0.3911	−0.3448	0.8533
$\frac{3}{2}$	0.0	0.0	−0.1358	0.9907
	0.0003	0.0	−0.1514	0.9885
$\frac{5}{2}$	0.0	0.0	0.0	1.0000
	0.0008	0.0	0.0	1.0000
$\frac{1}{2}$	0.0	0.7777	0.3671	0.5103
	0.0017	0.8596	0.1943	0.4726
$\frac{1}{2}$	0.0	−0.4887	0.8637	0.1233
	0.0016	−0.3288	0.9183	0.2204
$\frac{3}{2}$	0.0	0.0	0.9907	0.1358
	0.0005	0.0	0.9885	0.1514
$-E=40.842$	$Q_2=5.602$	$Q_4=4.346$	$\lvert C_0\rvert^2=1.0000$	
40.976	5.555	4.348	0.9898	

k	γ_k	$s^k_{1/2}$	$d^k_{3/2}$	$d^k_{5/2}$
		^{32}S		
		0.9951	0.3261	2.6787
		0.9783	0.4098	2.6113
$\frac{3}{2}$	1.0000	0.0	−0.1805	0.9836
	0.9877	0.0	−0.1695	0.9855
$\frac{1}{2}$	1.0000	0.0831	0.5319	0.8427
	0.9918	0.1638	0.5005	0.8501
$\frac{1}{2}$	1.0000	0.9941	−0.1031	−0.0330
	0.9871	0.9818	−0.1670	−0.0908
$\frac{5}{2}$	1.0000	0.0	0.0	1.0000
	0.9201	0.0	0.0	1.0000
$\frac{3}{2}$	0.0	0.0	0.9836	0.1805
	0.0967	0.0	0.9855	0.1695
$\frac{1}{2}$	0.0	0.0694	0.8405	−0.5373
	0.0161	0.0965	0.8495	−0.5187
$-E=222.965$	$Q_2=-0.546$	$Q_4=-1.440$	$\lvert C_0\rvert^2=1.0000$	
225.265	−0.547	−1.523	0.7744	

k	γ_k	$s^k_{1/2}$	$d^k_{3/2}$	$d^k_{5/2}$
		^{24}Mg		
		0.1966	0.1684	1.6351
		0.2034	0.2538	1.5427
$\frac{1}{2}$	1.0000	−0.4434	−0.3207	0.8370
	0.9953	−0.4414	−0.3090	0.8424
$\frac{3}{2}$	1.0000	0.0	−0.2561	0.9667
	0.8598	0.0	−0.2567	0.9665
$\frac{1}{2}$	0.0	0.3753	0.7816	0.4983
	0.1362	0.2598	0.8546	0.4496
$\frac{5}{2}$	0.0	0.0	0.0	1.0000
	0.0055	0.0	0.0	1.0000
$\frac{1}{2}$	0.0	0.8140	−0.5350	0.2262
	0.0005	0.8589	−0.4173	0.2970
$\frac{3}{2}$	0.0	0.0	0.9667	0.2561
	0.0027	0.0	0.9665	0.2567
$-E=91.994$	$Q_2=6.346$	$Q_4=-4.207$	$\lvert C_0\rvert^2=1.0000$	
94.442	6.451	−2.811	0.7103	

k	γ_k	$s^k_{1/2}$	$d^k_{3/2}$	$d^k_{5/2}$
		^{24}Mg		
		0.0	0.3222	1.6778
		0.0193	0.3072	1.6734
$\frac{5}{2}$	1.0000	0.0	0.0	1.0000
	0.9864	0.0	0.0	1.0000
$\frac{3}{2}$	1.0000	0.0	0.5676	0.8233
	0.9026	0.0	0.5657	0.8246
$\frac{1}{2}$	0.0	0.5352	−0.0676	0.8420
	0.0823	0.4444	−0.0748	0.8927
$\frac{3}{2}$	0.0	0.0	0.8233	−0.5676
	0.0209	0.0	0.8246	−0.5657
$\frac{1}{2}$	0.0	0.7161	−0.4925	−0.4946
	0.0061	0.6281	−0.6846	−0.3700
$\frac{1}{2}$	0.0	0.4481	0.8677	−0.2151
	0.0015	0.6388	0.7251	−0.2572
$-E=88.888$	$Q_2=-4.360$	$Q_4=-3.100$	$\lvert C_0\rvert^2=1.0000$	
90.394	−4.345	−2.225	0.7781	

TABLE I *(Continued)*

k	γ_k	$s^k_{1/2}$	$d^k_{3/2}$	$d^k_{5/2}$
		^{28}Si		
		0.4652	0.8146	1.7203
		0.4508	0.8151	1.7340
$\frac{1}{2}$	1.0000	−0.5514	−0.1300	0.8241
	0.9992	−0.5414	−0.1345	0.8299
$\frac{3}{2}$	1.0000	0.0	−0.3431	0.9393
	0.9978	0.0	−0.3408	0.9402
$\frac{1}{2}$	1.0000	0.4014	0.8246	0.3986
	0.9880	0.3978	0.8286	0.3938
$\frac{5}{2}$	0.0	0.0	0.0	1.0000
	0.0098	0.0	0.0	1.0000
$\frac{1}{2}$	0.0	−0.7313	0.5506	−0.4026
	0.0029	−0.7407	0.5434	−0.3951
$\frac{3}{2}$	0.0	0.0	0.9393	0.3431
	0.0023	0.0	0.9402	0.3408
$-E = 141.149$	$Q_2 = 7.589$	$Q_4 = -2.912$	$\lvert C_0\rvert^2 = 1.0000$	
141.485	7.554	−2.860	0.9700	
		^{36}Ar		
		0.9999	1.0321	2.9680
		0.9896	1.0903	2.9172
$\frac{1}{2}$	1.0000	−0.3517	−0.0556	0.9344
	0.9976	−0.3506	−0.0552	0.9349
$\frac{3}{2}$	1.0000	0.0	−0.1789	0.9839
	0.9935	0.0	−0.1758	0.9844
$\frac{5}{2}$	1.0000	0.0	0.0	1.0000
	0.9561	0.0	0.0	1.0000
$\frac{1}{2}$	1.0000	0.9156	0.1871	0.3558
	0.9880	0.9161	0.1872	0.3546
$\frac{1}{2}$	1.0000	−0.1946	0.9808	−0.0149
	0.9971	−0.1946	0.9808	−0.0151
$\frac{3}{2}$	0.0	0.0	0.9839	0.1789
	0.0648	0.0	0.9844	0.1758
$-E = 306.771$	$Q_2 = 2.684$	$Q_4 = 0.287$	$\lvert C_0\rvert^2 = 1.0000$	
308.322	2.692	0.164	0.8697	

k	γ_k	$s^k_{1/2}$	$d^k_{3/2}$	$d^k_{5/2}$
		^{28}Si		
		0.6349	0.6506	1.7147
		0.6185	0.6075	1.7740
$\frac{5}{2}$	1.0000	0.0	0.0	1.0000
	0.9968	0.0	0.0	1.0000
$\frac{1}{2}$	1.0000	0.7968	−0.2784	0.5363
	0.9978	0.7868	−0.2694	0.5553
$\frac{3}{2}$	1.0000	0.0	0.7570	0.6535
	0.9923	0.0	0.7300	0.6835
$\frac{3}{2}$	0.0	0.0	−0.6535	0.7570
	0.0076	0.0	−0.6835	0.7300
$\frac{1}{2}$	0.0	−0.3913	0.4385	0.8091
	0.0034	−0.1651	0.7751	0.6099
$\frac{1}{2}$	0.0	0.4604	0.8545	−0.2405
	0.0019	0.5947	0.5715	−0.5654
$-E = 143.770$	$Q_2 = -7.870$	$Q_4 = 0.882$	$\lvert C_0\rvert^2 = 1.0000$	
144.199	−7.714	0.639	0.9740	
		^{36}Ar		
		0.8443	1.3217	2.8341
		0.8391	1.3260	2.8347
$\frac{5}{2}$	1.0000	0.0	0.0	1.0000
	0.9992	0.0	0.0	1.0000
$\frac{3}{2}$	1.0000	0.0	0.1832	0.9831
	0.9985	0.0	0.1857	0.9826
$\frac{1}{2}$	1.0000	0.5818	0.1193	0.8046
	0.9991	0.5784	0.1151	0.8076
$\frac{1}{2}$	1.0000	0.7112	−0.5545	−0.4321
	0.9970	−0.7102	0.5581	0.4291
$\frac{3}{2}$	1.0000	0.0	0.9831	−0.1832
	0.9937	0.0	0.9826	−0.1857
$\frac{1}{2}$	0.0	0.3946	0.8236	−0.4074
	0.0123	0.4013	0.8217	−0.4046
$-E = 308.654$	$Q_2 = -3.839$	$Q_4 = -0.996$	$\lvert C_0\rvert^2 = 1.0000$	
308.843	−3.782	−0.964	0.9754	

C. Results and Discussion

Table I summarizes the main results of this study. Besides the energies, orbitals, and configuration coefficients, we also calculated the strengths of the spherical single-particle levels, usually measured in stripping or pickup reactions. They are given for each basis state j by the one-body density matrix elements in the basis representation:

$$\gamma_j = \sum_k \langle jk|\gamma|jk\rangle . \tag{26}$$

Also shown in Table I are the occupation probabilities of the MCSC orbitals, γ_λ, for occupied orbitals. The shape of an intrinsic state is characterized by its quadrupole and hexadecapole moments, Q_2 and Q_4, defined by the dimensionless matrix elements

$$Q_L = \left(\frac{4\pi}{2L+1}\right)^{1/2} \sum_{i=1}^{A} \left(\frac{r_i}{b}\right)^L Y_{L0}(\hat{r}_i) \quad , \tag{27}$$

or alternatively by the distortion parameters β_2 and β_4, which, for axially symmetric deformations, are defined by

$$\beta_L = \left(\frac{4\pi}{2L+1}\right)^{1/2} \frac{Q_L}{AR_L} , \tag{28}$$

where

$$R_L = \frac{1}{A} \left\langle \sum_{i=1}^{A} \left(\frac{r_i}{b}\right)^L \right\rangle . \tag{29}$$

The effects of the correlations are most clearly seen in the dispersion of the occupation probabilities γ_λ across the Fermi surface, and also in the redistribution of the single-particle strengths γ_j in the spherical-basis states. These effects are largest in ^{24}Mg and ^{32}S, and almost imperceptible in ^{20}Ne (Table I and Fig. 2). The amount of dispersion of the occupation density depends on the correlations allowed to the system, which in turn are determined by the HF single-particle energy gap. In ^{36}Ar, for example, the HF calculations predict a stable oblate solution which is lower than the prolate solution by 3 MeV in energy and has a single-particle energy gap twice as large as the gap in the prolate spectrum. For this reason the former solution should be preferred. However, with the introduction of the correlations, the prolate solution gives a larger energy gain than the oblate solution, bringing the two states together in energy.

Two competing effects contribute to the net energy gain: the dispersion of particles to levels of lower binding energies, and the rearrangement of particles for a more stable configuration. The energy gain from the latter effect, however, more than compensates for the loss from the former. A notable feature of our results is that, with the introduction of the correlations, the prolate states

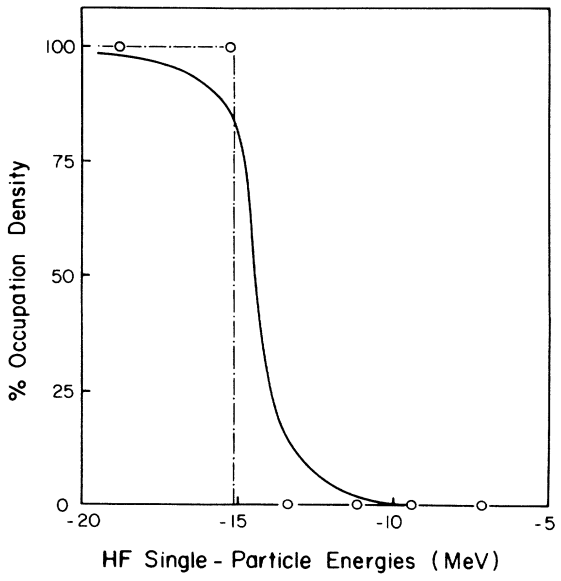

FIG. 2. Occupation density of the single-particle orbits of ^{24}Mg in the HF approximation (dot-dash curve) and the MCSC approximation (solid curve).

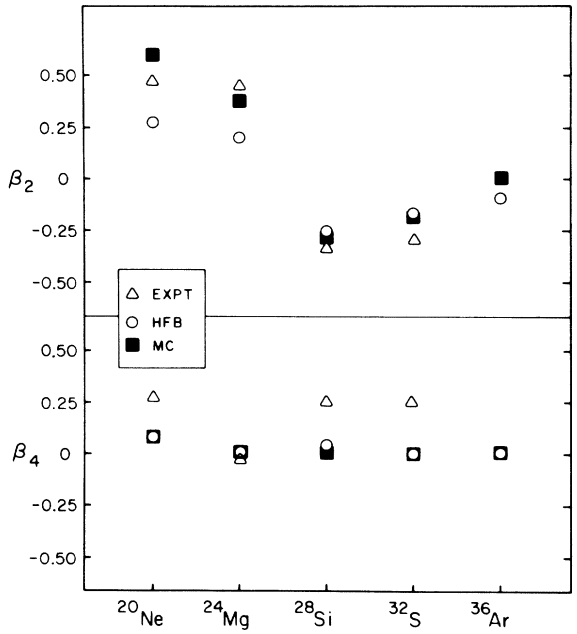

FIG. 3. The distortion parameters β_2 and β_4 as calculated in the MCSC and HFB (Ref.12) methods, and as obtained from experimental data (Ref. 19). The HF values are very close to the corresponding MCSC values. For β_2: 0.634, 0.359, −0.297, −0.002, and 0.061; for β_4: 0.079, −0.39, 0.006, −0.006, and 0.001 for Ne, Mg, Si, S, and Ar, respectively.

TABLE II. Correlation energies in MeV for the most stable solutions as given by method A of Ref. 16 and by the MCSC method.

	Ne	Mg	Si	S	Ar
Method A	0.130	2.254	0.417	2.186	0.192
MCSC	0.134	2.448	0.430	2.300	0.189

record a larger energy gain than the corresponding oblate states and thus become relatively more stable. For example, the respective energy gains for prolate and oblate states are 2.4 and 1.5 MeV in ^{24}Mg, and 1.6 and 0.2 MeV in ^{36}Ar. This tendency toward a higher symmetry is a well-established feature of the pairing correlations in heavy as well as in light deformed nuclei. Bar-Touv *et al.*[12] have shown that the isospin pairing restored axial symmetry to ^{24}Mg, thus making the wave function more consistent with experimental data.

In Fig. 3 we compare our calculated values of the distortion parameters β_2 and β_4 with the values obtained from an analysis of inelastic scattering data.[19] Also shown in this figure are the results of Bar-Touv *et al.*'s calculation.[12]

All parameters discussed so far, with the exception of the energy, depend on single-particle operators and are rather insensitive to the correlations under study. A more stringent test of the wave functions obtained in this work would involve the calculations of the physical nuclear states and the rates of electromagnetic transition between these states.

Recently Padjen and Ripka[13] proposed two methods of estimating the effects of correlations on the ground-state energy. In their method A, one would diagonalize the Hamiltonian H in the space of the excited configurations; the eigensolutions would subsequently be used to calculate the energy shift of the ground state. Method B is a fully self-consistent scheme for calculating the correlation energy defined in terms of excitations of the nucleons; it bypasses the construction of an intrinsic wave function. The authors reported that the two methods actually yielded very similar results. Using our parameters and configurations we have carried out a calculation according to method A. The results are listed in Table II, and show that again the simpler method A is close to the MCSC method, at least under the assumptions made in this paper.

In fact our MCSC calculations (Table I) yield smaller energy gains than those reported in Ref. 16; this disagreement may stem from the choice of a different Hamiltonian, but a more probable reason may lie in the different choice of configurations. Our set includes mostly configurations containing time-reversed pairs, and hence is more restrictive. For this same reason our results are close to the HFB results, as is apparent, for example, in Fig. 3.

IV. CONCLUSION

We have formulated a variational method of obtaining correlated intrinsic wave functions. We have investigated general features of the resulting field in light deformed nuclei assuming, in this first attempt, 2p-2h correlations and a truncated-basis space. As generally expected, the ^{20}Ne nucleus is well described by the HF static field; all other nuclei considered are more or less affected by the dynamical correlations, leading to a greater stability both in terms of the binding energy and the shape symmetry.

The formalism presented here offers a versatile and powerful method for the study of deformed nuclei. Many questions, however, remain open. The immediate task is to investigate the importance of other types of correlations; however, a full-blown MCSC calculation would be an extravagance; a preliminary perturbative calculation could decide which configurations to retain. The excited intrinsic states given by the higher-energy solutions of Eq. (7a) should also deserve a more careful study. And, finally, the value of the MCSC method can be fully appreciated only when an angular momentum projection is performed on the calculated wave function, and properties of the resulting physical states compared with experimental data.

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Outgoing Alpha-Channel Resonances in Reactions Having ^{17}F as an Intermediate System

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Excitation functions for the reactions ^{14}N(^{3}He, α)^{13}N and ^{14}N(^{3}He, p)^{16}O have been measured in the energy range 3.75 to 10.75 MeV and 5.5 to 10.5 MeV, respectively. These data have been compared with those for the ^{16}O(p,p')^{16}O and the ^{16}O(p, α)^{13}N reactions which also proceed through the same ^{17}F intermediate system. The results of this comparison support the hypothesis of α-like cluster resonances in the outgoing reaction channel.

1. INTRODUCTION

Resonances in composite-particle outgoing reaction channels have been postulated by Wildermuth and Carovillano in 1961.[1] In their picture, starting from the capture of the bombarding particle, the compound nuclear system passes through different cluster structures. The lifetime of these clusters can be of sufficient duration for a giant-resonance structure to occur in the energy dependence of certain partial-decay cross sections. This is the case of the outgoing channels in α-particle scattering or (p, α) reactions; in effect Wildermuth discusses just the ^{16}O(p, α)^{13}N$_{g.s.}$ reaction, predicting resonance widths of the order of a few hundred keV.

Recent work of Gillet[2] has stressed the importance of quartet structures in the interpretation of nuclear excited states. One again expects resonances in the α channel at compound-system energies corresponding to these states. Whitehead and Foster[3] and Maxon[4] have reported the existence of resonances with widths of 1–2 MeV in the ^{16}O(p, α)^{13}N$_{g.s.}$ reaction for proton energies in the range from 6 to 20 MeV. Recent measurements performed at the Milan cyclotron[5] on the same reaction show resonance structures in the excitation functions also at higher proton energies. It seemed, therefore, interesting to investigate experimentally to what extent the origin of these resonances is associated with the outgoing channel.

To this end we compare the ^{16}O(p, α)^{13}N excitation function with that of the proton inelastic scattering on the same target[6] and with those of the ^{14}N(^{3}He, α)^{13}N and ^{14}N(^{3}He, p)^{16}O reactions which also proceed via the same fluorine-17 intermediate system. The helium-3 data used in this comparison have been taken as part of this investigation and are reported in Sec. 3. If the resonances in the (p, α) excitation function are characteristic