Hybrid symmetry-conserving variational procedure for nuclear structure calculations

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A recently proposed hybrid variational procedure for nuclear structure calculations is improved and reformulated in a way that allows for going beyond the mean-field approximation. The numerical feasibility of the resulting approach is tested by applying it in the *s-d* shell. Selected examples demonstrate that the procedure works equally well for odd-mass and even-mass nuclei, giving solutions that rapidly converge to the exact ones.

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I. INTRODUCTION

The natural framework for microscopic calculations of the structure of all but the lightest nuclei is the nuclear shell model. Its technology, known as shell-model configuration mixing (SCM), has developed to the point that complete $0\hbar\omega$ calculations are possible within the whole *s-d* shell and even for some nuclei of the *f-p* shell [1]. Accordingly, high quality forces have been fitted to reproduce a wide variety of nuclear properties [2,3]. At the same time, the situation is not so optimistic as it may seem at first glance. The major problem of the shell-model configuration mixing method is that the number of configurations increases drastically with the number of single-particle basis states. Increasing the size of the single-particle basis rapidly renders complete SCM calculations not only impractical but impossible. One is then forced to choose between using Monte Carlo methods [4] or truncating, in some way, the complete SCM space. The question of how such a truncation is to be performed in order to maximize the correlations included with as few configurations as possible is at the crux of all microscopic nuclear structure calculations. There have been various approaches to this truncation, ranging from the extreme single-configuration approximation known as the Hartree-Fock method [5] to the more recent many-determinant VAMPIR approach [6]. Both of these are basically variational approaches, in which one or several particle or quasiparticle mean fields are consistently determined and then used in a subsequent diagonalization of the residual interaction. Such procedures have the attractive feature that the truncation of the SCM space is dictated by the dynamics of the many-body system itself, rather than introduced *ad hoc*. On the other hand, the price that must be paid in order to account for a large part of the complete SCM dynamics using only a moderate number of configurations is the nonconservation of certain symmetries of the Hamiltonian. Those that are violated most often are angular momentum and parity conservation, and sometimes also particle number conservation. Thus, in order to obtain physical information, one needs to restore the broken symmetries by using appropriate projection operators, either before or after variation of the intrinsic states [5]. These projection operators, however, introduce technical complications which result in orders of magnitude increases in the necessary numerical effort. In order to end up with a manageable problem, one is then forced to impose restrictions on the variational space. A whole hierarchy of various possible ways of doing this was proposed about ten years ago [7]. All are based on symmetry-projected Hartree-Fock-Bogolyubov-type (HFB) quasiparticle Slater determinants, which are allowed to break as many symmetries as possible. Since then, almost all of the resulting approaches have been used in realistic applications, yielding very encouraging results [8]. The favorite among them, known as (excited) FED VAMPIR [6], uses a few symmetry-projected HFB-type states, determined via variation after symmetry projection (VAP), to approximate each individual state of the many-body system. To ensure the numerical feasibility of the method, one still has to enforce axial and time-reversal symmetry on the trial HFB states. This restriction makes odd-mass nuclei inaccessible with the latest numerical realization of the method. In addition, some states of even-even nuclei cannot be described in this way, namely, those dominated by the so-called "missing configurations," as discussed in [8]. Although these shortcomings are of a technical rather than a fundamental nature, it is very doubtful that they can be overcome in the near future.

In the present work, another possibility is explored. Instead of imposing axial symmetry and allowing particle number violation in the trial state, mean fields of general shape are allowed but the particle number is fixed. In such an approach, the *explicit* inclusion of pairing correlations is given up in favor of axial symmetry violation. This approach is motivated by our previous results, indicating the importance of relaxing the axial symmetry

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restriction [9,10]. Since full angular momentum projection, even in its optimized form [9], requires threefold integration and thus is too time consuming to be carried out before variation, a hybrid treatment of the rotational invariance is adopted. Compared to [10], the present work contains two important improvements: (a) It goes beyond the mean-field approximation by permitting several symmetry-projected intrinsic states for the description of each state of interest; and (b) together with the exact axial symmetry projection an approximate full rotational symmetry projection before variation is carried out. Since, as in the FED VAMPIR, several symmetry projected mean fields are used to describe each individual state of the correlated system, it is clear that the method should in principle be able to reproduce the exact solutions of the SCM.

The presentation is organized as follows. In Sec. II, the basics of the approach are given. Some of the information therein can be found in the literature (e.g., [11]) and is included here to make the presentation self-contained. The variational procedure is explained in some detail in Sec. III. Section IV contains results of some selected applications of the approach to realistic nuclear systems in the *s-d* shell. Finally, a discussion of the results and the principal conclusions are collected in Sec. V.

II. BASIC FORMALISM

The intrinsic states of our model are normalized products of proton and neutron Slater determinants, similarly to the so-called "multiconfiguration Hartree-Fock" [12]. For simplicity, we shall assume one type of particle in what follows. Thus, an N-particle intrinsic state in an M-dimensional single-particle basis is constructed as ($|-\rangle$ is the vacuum)

$$|\Phi\rangle = \prod_{i=1}^{M} a_i^\dagger |-\rangle \ . \tag{2.1}$$

The creation operators $a^\dagger$ are built by using some fixed M-dimensional single-particle basis (e.g., harmonic oscillator or Woods-Saxon basis) with creation operators $c^\dagger$:

$$a_i^\dagger = \sum_{a=1}^{M} A_{ai} c_a^\dagger \qquad (i = 1, 2, \ldots, N) \ . \tag{2.2}$$

The rectangular matrix A is chosen such that the proper fermionic anticommutation relation for the a and $a^\dagger$ operators is guaranteed:

$$\sum_{a=1}^{M} A_{ai}^* A_{aj} = \delta_{ij} \ . \tag{2.3}$$

Note that one does not need to specify the single-particle states that are not occupied in (2.1). When no further restrictions on A are imposed, the state (2.1) represents the most general mean field (Slater determinant) within the chosen single-particle basis.

In order to be able to use the above states, one needs the following "building" blocks. First, consider the overlap between two intrinsic states $|L\rangle$ and $|R\rangle$. Using (2.1), one obtains

$$\begin{aligned}\langle L|R\rangle &= \left\langle - \left| \prod_{i=1}^{N} a_i(L) \prod_{j=1}^{N} a_j^\dagger \right| - \right\rangle \\ &= \sum_{ab=1}^{M} A_{1a_1}^\dagger(L) \cdots A_{Na_N}^\dagger(L) A_{1b_1}(R) \cdots A_{Nb_N}(R) \langle - | c_{a_1} \cdots c_{a_N} c_{b_1}^\dagger \cdots c_{b_N}^\dagger | - \rangle \\ &= \det\{A^\dagger(L) A(R)\} \equiv \det \mathcal{N}(L,R) \ ,\end{aligned} \tag{2.4}$$

where the last row defines the matrix $\mathcal{N}$. The next thing of interest is the transitional one-body density matrix. An expression for it can be obtained by taking into account that $a_j|\Phi\rangle = 0$ for $j > N$ and inverting (2.2). One has

$$\begin{aligned}\rho_{ba}(L,R) \equiv \langle L|c_a^\dagger c_b|R\rangle = \sum_{\alpha\beta=1}^{N} A_{\alpha a}^\dagger(L) A_{b\beta}(R) \langle L|a_\alpha^\dagger a_\beta|R = \sum_{\alpha\beta=1}^{N} A_{\alpha a}^\dagger(L) A_{b\beta}(R) \frac{\partial det\mathcal{N}(L,R)}{\partial \mathcal{N}_{\alpha\beta}(L,R)} \\ = \langle L|R\rangle \{A(R)\mathcal{N}^{-1}A^\dagger(R)\}_{ba} \ .\end{aligned}$$

In the last row the overlap $\langle L|R\rangle$ is assumed not to vanish. A similar calculation provides us with a relation between the two-body and one-body transitional density matrices:

$$\langle L|c_a^\dagger c_b^\dagger c_d c_c|R\rangle = \langle L|R\rangle \{\rho_{db}(L,R)\rho_{ca}(L,R) - \rho_{da}(L,R)\rho_{cd}(L,R)\} \ .$$

The logic of building up the three- and more-particle overlaps using the one-body transitional density matrix should now be obvious.

The intrinsic states discussed above have, in general, neither definite total angular momentum nor definite third projection of the angular momentum. In order to obtain physical states, the rotational symmetry must be restored by projection [5]. In this work we use the opti-

mal finite sum representation [9] of the three-dimensional Hill-Wheeler projection operator, involving Gauss-Jacobi and Gauss-Chebishev integration formulas. More specifically, the axial symmetry projector on $\hat{J}_z = M$ is given by

$$\hat{P}_M = \frac{\pi}{2L} \sum_{j=1}^{L} e^{iM\phi_j} \hat{R}_z(\phi_j), \quad \phi_j = \pm \frac{2j+1}{2L} \pi \ , \quad (2.5)$$

and the full angular momentum projector by

$$\hat{P}^J_{MM} = \sum_{l,j=1}^{L} \sum_{k=1}^{L'} e^{iM(\alpha_l + \gamma_j)} \cos^{-2M} \left(\frac{\beta_k}{2} \right) \times w_k \hat{R}(\alpha_l, \beta_k, \gamma_j) \ , \quad (2.6)$$

where

$$\alpha_j, \gamma_j = \pm \frac{(2j-1)}{2L} \pi, \quad \beta_k = \arccos(\eta_k) \ ,$$

$$w_k = \mathcal{M} \{ P'_{L'}{}^{(0,2M)}(\eta_k) P^{(0,2M)}_{L'+1}(\eta_k) \}^{-1} .$$

$\mathcal{M}$ is an overall normalization factor, and η_k are the zeros of the Jacobi polynomial $P^{(0,2M)}_{L'}(\eta_k)$. The action of the projector (2.6) on a Slater determinant is simple; one only needs the action of the rotation $\hat{R}(\alpha, \beta, \gamma)$ on (2.1). It is given by

$$\hat{R}(\Omega)|\Phi\rangle = \prod_{i=1}^{N} \hat{R}(\Omega) a_i^\dagger \hat{R}^\dagger(\Omega)|-\rangle \ ,$$

$$\hat{R}(\Omega) a_i^\dagger \hat{R}^\dagger(\Omega) = \sum_{a=1}^{M} A_{ai}(\Omega) c_a^\dagger \ ,$$

$$A_{ai}(\Omega) = \sum_{b=1}^{M} \delta_{AB} D^{j_a}_{m_b m_a}(\Omega) A_{bi} \ .$$

Equipped with the above formulas, we can proceed to discussing our variational procedure.

III. VARIATIONAL PROCEDURE

Consider a Hamiltonian consisting of one- and two-body parts:

$$\hat{H} = \sum_a \epsilon_a c_a^\dagger c_a + \frac{1}{4} \sum_{abcd} \mathcal{V}_{abcd} c_a^\dagger c_b^\dagger c_c c_d \ . \quad (3.1)$$

In what follows, we shall restrict our attention to the action of the above operator on states of definite particle number, i.e., on eigenstates of $\hat{N} = \sum_a c_a^\dagger c_a$. This makes it possible to incorporate the one-body term of (3.1) into its two-body term:

$$\hat{H} = \frac{1}{4} \sum_{abcd} V_{abcd} c_a^\dagger c_b^\dagger c_c c_d \ ,$$

$$V_{abcd} = \mathcal{V}_{abcd} + \frac{1}{N-1} (\epsilon_a + \epsilon_b)(\delta_{ac}\delta_{bd} - \delta_{ad}\delta_{bc}) \ .$$

This somewhat simpler form of the Hamiltonian is used in the actual calculations.

Our model space for the diagonalization of the above Hamiltonian is spanned by several intrinsic Slater determinants, projected on good angular momentum. This implies many-body wave functions of the kind

$$|\psi_{JJ}\rangle = \sum_k g_k \hat{P}^J_{JJ} |\phi_k\rangle \ . \quad (3.2)$$

The intrinsic states $|\phi_k\rangle$ and the mixing coefficients g_k are to be determined variationally. This means that, ideally, one has to solve

$$\delta \frac{\langle \psi_{JJ}|\hat{H}|\psi_{JJ}\rangle}{\langle \psi_{JJ}|\psi_{JJ}\rangle} = 0 \ . \quad (3.3)$$

In all cases of practical interest, however, the triple integration involved in the projection operator $\hat{P}^J_{JJ}$ makes the variation after projection intractable. Therefore, we resort to a pedestrian version of (3.3)—the so-called hybrid treatment of the rotational symmetry [10]. Within this scheme, the axial symmetry of the intrinsic states is restored before the variation, while the full angular momentum projection is carried out after having determined the intrinsic states. Since our goal is to approximate (3.3) as close as possible, we employ an approximate full angular momentum projection before the variation. This is done by modifying the Hamiltonian $\hat{H}$ in the way proposed by Kamlah years ago [13,5]:

$$\hat{H}(\lambda) = \hat{H} - \lambda \hat{J}^2 \ .$$

Thus our intrinsic Slater determinants are determined by the requirement

$$\delta \frac{\langle \psi_J|\hat{H}(\lambda)|\psi_J\rangle}{\langle \psi_J|\psi_J\rangle} = 0 \ , \quad (3.4)$$

where the variational states are eigenstates of $\hat{J}_z$:

$$|\psi_J\rangle \quad = \sum_k g_k \hat{P}_J |\phi_k\rangle \ .$$

In the original Kamlah approach the value of λ is given by a complicated expression involving the expectation value of the three-body operator $\hat{H}\hat{J}^2$ [5]. Instead of evaluating λ in this way, we determine its value by an additional one-dimensional minimization.

Let us now summarize our hybrid variational procedure: Suppose we have $n-1$ intrinsic Slater determinants. The next, nth, one is determined by solving (3.4) with the variation involving the nth Slater determinant only but all mixing coefficients for some chosen value of λ. The resulting Slater determinant together with the $n-1$ fixed ones is used for solving (3.3) where only the mixing coefficients g_k are varied. It is well known that variation of the mixing coefficients is equivalent to diagonalizing $\hat{H}$ in the nonorthonormal basis of the n projected Slater determinants. After this is done, λ is modified and the above is repeated until a minimum for the lowest eigenvalue is found. In general, all n Slater determinants should be varied simultaneously. It has been argued, however, that such a fine tuning barely changes

the final results [6]; we have independently arrived at the same conclusion: The effort needed to vary simultaneously all determinants, compared to the improvement of the results, overrules such a procedure.

In order to complete the description of the variational procedure, we have to discuss the variation of a Slater determinant. Since, as a result of (2.3), the elements of the matrix A from (2.2) are not independent, they cannot be directly used as variational parameters. Therefore, we take the representation of a general unitary matrix

$$A = (1 + iX)(1 - iX)^{-1} , \tag{3.5}$$

where X is a Hermitian matrix, and use the elements of the upper triangle of X as independent variables. Because of the redundancy of the last $M - N$ columns of A, their number is certainly greater than the minimal number of parameters needed to specify a Slater determinant. We nevertheless adopt the representation (3.5) because of its generality and because it is easily invertable, in contrast to the usual one of Thouless. Now the variation of a Slater determinant can be written as

$$|\delta\Phi\rangle = \delta \prod_{i=1}^{N} \sum_{a=1}^{M} A_{ai} c_a^\dagger |-\rangle$$
$$= \sum_{ab=1}^{M} \delta A_{ab} c_a^\dagger a_b |\Phi\rangle = \sum_{abc=1}^{M} \delta A_{ac} A_{bc}^* c_a^\dagger c_b |\Phi\rangle .$$

From (3.5), it is easily seen that $\delta A A^\dagger$ is given by $\frac{i}{2}(1 + A)\delta X(1 + A^\dagger)$. Thus, we finally have

$$|\delta\Phi\rangle = \frac{i}{2} \sum_{ab=1}^{M} \{(1 + A)\delta X(1 + A^\dagger)\}_{ab} c_a^\dagger c_b |\Phi\rangle .$$

IV. NUMERICAL APPLICATIONS

For the first applications of the procedure described above, we have chosen only a $1s0d$ single-particle basis. There is a standard effective force for this space [2], which is also used in this work.

We first consider the ground-state band of the even-odd nucleus ^{21}Ne up to $J = \frac{11}{2}$. Addressing this relatively "simple" problem, we expect our approach to rapidly converge to the corresponding SCM solutions, even with λ fixed to 0. The results of our calculations together with the exact SCM energies are presented in Fig. 1. All energies are with respect to a doubly magic ^{16}O core. The convergence to the exact results is obvious, but what is more striking is that with only three to four intrinsic states an accuracy of 0.3% in the spectrum is achieved. Especially nicely reproduced are the excitation energies, the errors being mainly due to an overall shift of the spectrum upwards. As we shall see later, this same feature persists in all our calculations.

As a next example, the nucleus ^{29}Si near the middle of the shell is considered. The m-scheme shell-model configuration mixing for the ground state of this nucleus has to deal with 80 115 Slater determinants. Within our approach, we try to do the same job with only one or two determinants, selected by the dynamics of the system. Figure 2 shows the results of various approaches to the energies of the lowest four members of the ground-state band of ^{29}Si. From left to right we have the exact diagonalization results (SCM), variation after full angular momentum projection (VAP), the hybrid procedure from (3.4) with one intrinsic Slater determinant (CHT), and the same but with λ fixed to 0 (HT). The crucial role of the approximate full angular momentum projection before variation by introducing $\hat{J}$ as a constraint is clearly seen.

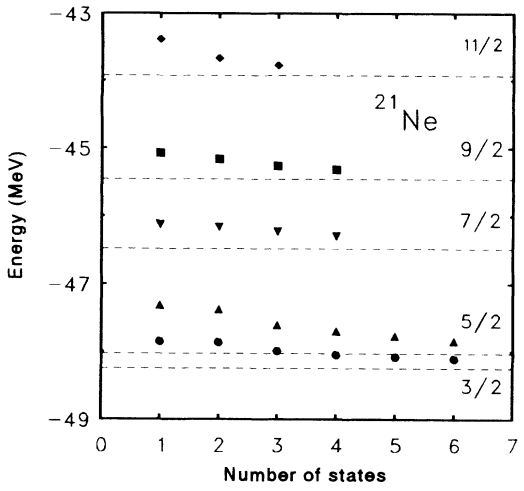

FIG. 1. Energies of five members of the ground-state band of ^{21}Ne, calculated with $\lambda = 0$. The dashed lines indicate the energies of the corresponding exact SCM solutions.

To judge the quality of the approximation, however, excitation energies alone are not enough. Further observables that test different aspects of the wave functions need also to be considered. Recently, the spin structure function of ^{29}Si, which is of interest in astrophysics, has been calculated within the same shell-model space and using the same force [14]. Figure 3 shows a comparison of the SCM spin structure function with those ob-

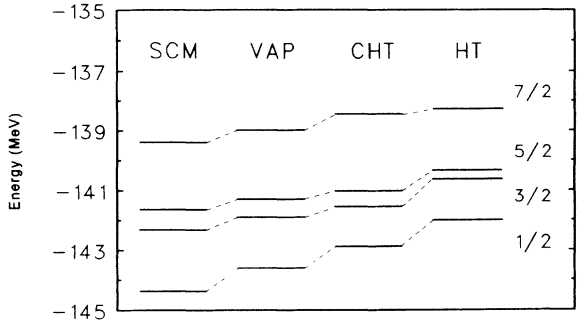

FIG. 2. Results of various approaches for the lowest four states of the ground-state band in ^{29}Si. Notations are explained in the text.

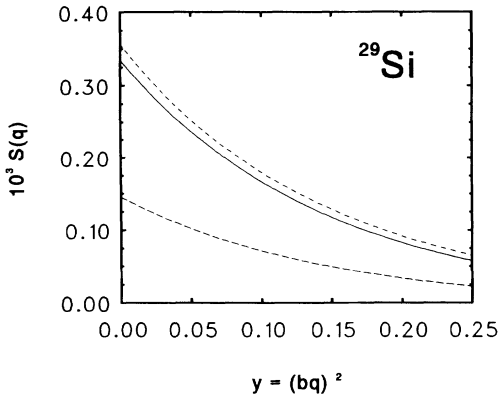

FIG. 3. Spin structure functions of the ground state of ^{29}Si as given by exact SCM [14] (solid line), CHT with one intrinsic state (long-dashed line), and CHT with two intrinsic states (short-dashed line). b is the oscillator parameter of the basis, q is the momentum transfer.

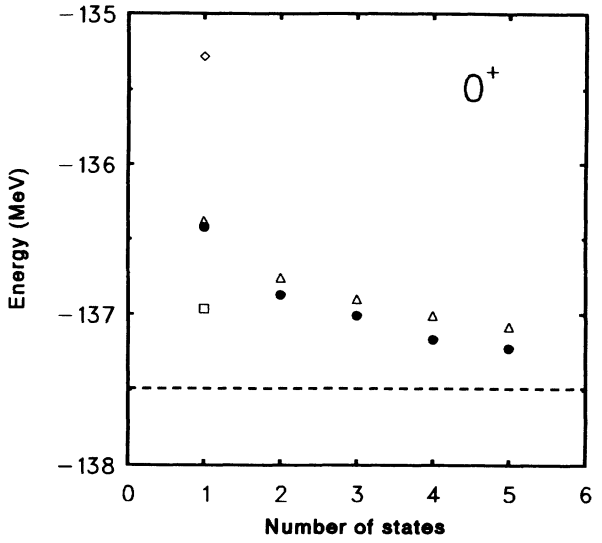

FIG. 4. Energy of the ^{29}Si ground state as obtained by the various approaches: bare hybrid treatment with $\lambda = 0$ (◇), FED VAMPIR (△), hybrid treatment with $\lambda \neq 0$ (●), and full VAP (□). The dashed line indicates the position of the exact SCM solution.

tained with our approach using one and two intrinsic Slater determinants. Already with two intrinsic states we achieve a very good description of the spin structure of the ground state. Related to the spin is the magnetic moment of the ground state. The measured magnetic moment of ^{29}Si is $-0.55\mu_N$, well above the corresponding Schmidt value of $-1.9\mu_N$. The quenching of the magnetic moment is usually associated with two-body correlations in the ground state. Thus, the (in)ability of an approximate scheme to account for this quenching is an indication of its (in)efficiency in describing such correlations. The exact SCM result is $-0.50\mu_N$; our approach gives $-0.36\mu_N$ with one intrinsic state and $-0.53\mu_N$ with two.

It is interesting to compare our hybrid symmetry-conserving procedure to the most powerful symmetry-conserving mean-field approach developed so far by the Tübingen group, the excited FED VAMPIR [6]. As noted earlier, this method is based on the mixing of axially symmetric Hartree-Fock-Bogolyubov (HFB) Slater determinants, projected on good proton and neutron numbers and angular momentum. The intrinsic HFB states are determined by a chain of variational calculations, similar to those described above. For the sake of comparison, we take the modified Wildenthal force and the corresponding single-particle energies from [6] and calculate the lowest 0^+, 2^+, and 4^+ states of ^{28}Si, mixing up to five intrinsic Slater determinants. The results of our calculations, together with those of the FED VAMPIR approach, are displayed in Figs. 4–6. Once again, the importance of the approximate full angular momentum projection before variation is clearly seen by comparing the results of the bare hybrid treatment to those of the constrained one. In the case of $J = 4$, the approximate full angular momentum projection turns out almost exact. In all cases, the hybrid procedure yields results that are equivalent to, or better than, those of the FED VAMPIR. As in the case of ^{29}Si, the whole spectrum is shifted upwards, but its shape is well reproduced. The excitation energies of the transitions $0^+ \rightarrow 2^+$ and $0^+ \rightarrow 4^+$ are plotted in Fig. 7, showing that two intrinsic states are enough to reproduce the spacing in the spectrum.

V. DISCUSSION AND CONCLUSIONS

In the present paper we have proposed and tested a hybrid symmetry-conserving variational procedure for nuclear structure calculations. The basic idea behind it

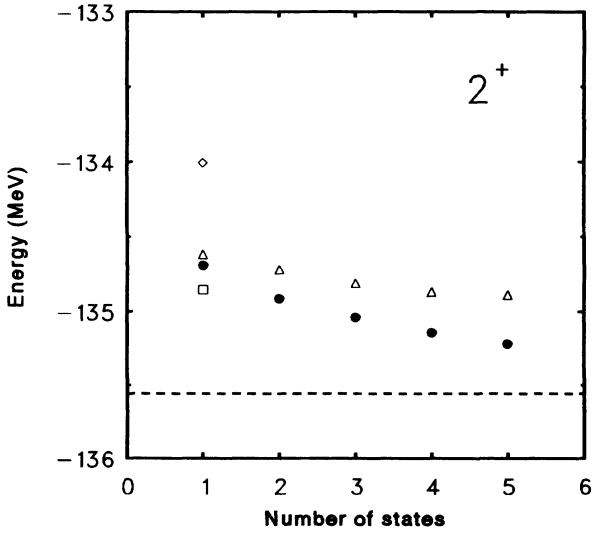

FIG. 5. Same as Fig. 4, but for the first 2^+ state.

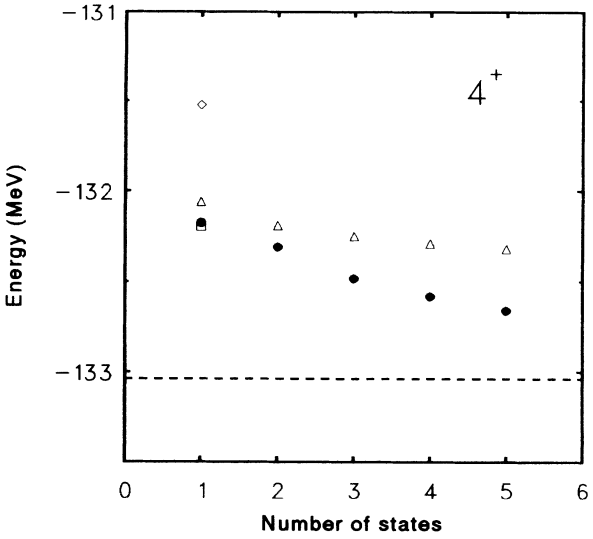

FIG. 6. Same as Fig. 4, but for the first 4^+ state.

is the mixing of variationally selected general deformed Slater determinants with partial restoration of rotational symmetry before and after the variation. Before variation, the axial symmetry is restored exactly and the full rotational symmetry approximately, using an approach similar to that proposed by Kamlah years ago. After the intrinsic states are determined, they are projected on good total angular momentum and then the Hamiltonian is diagonalized in the resulting nonorthonormal basis. Since the Slater determinants are themselves overcomplete in the many-body Hilbert space, it is clear that by increasing the number of intrinsic states the above procedure is capable of yielding exact eigenstates of the many-body Hamiltonian. Therefore, the relevant question is, how fast is the convergence to the exact eigenstates? The rate of convergence depends on how much of the important correlations can be accounted for by a single symmetry-projected intrinsic state. Which correlations are important depends on the two-body force, and

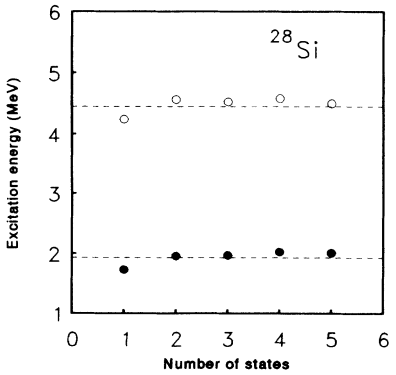

FIG. 7. Excitation energies for the $0^+ \rightarrow 2^+$ (•) and $0^+ \rightarrow 4^+$ (○) transitions. The dashed lines indicate the positions of the corresponding exact SCM solutions.

it is widely accepted that the most important components are the pairing and quadrupole-quadrupole ones. As discussed by Lipkin long ago [15], the only natural way to describe correlations using independent particle states is to allow them to break the symmetries of the Hamiltonian. The correlations due to pairing imply particle number violation, and those due to the quadrupole-quadrupole force imply deformation in the usual sense. In order to work with physical states, we need to restore the broken symmetries by projection. Unfortunately, for numerical reasons it is not possible to do this simultaneously for the particle number and the angular momentum. The standard compromise is to enforce axial symmetry and thus to work with axially symmetric HFB mean fields; this is the basis of the VAMPIR approach. In this work we have explored another possibility—enforcing particle number conservation and allowing general deformations of the mean fields. The results reported in the previous section suggest that trading particle number violation for axial symmetry violation is a good bargain. Since this comes as a bit of a surprise, let us try to understand how it comes about.

Consider for instance two particles moving in a single j shell and interacting with a pure pairing force. The exact ground-state wave function of this system is well known [5]:

$$|\mathrm{GS}\rangle = (j+\tfrac{1}{2})^{-\frac{1}{2}} \sum_{m>0} c_m^\dagger c_{-m}^\dagger |-\rangle \ .$$

On the other hand, a general Slater determinant for two particles projected on good axial symmetry is given by

$$\begin{aligned} |\Phi_0\rangle &= \hat{P}_0 a_1^\dagger a_2^\dagger |-\rangle \\ &= \sum_{m>0} (A_{m1}A_{-m2} - A_{-m1}A_{m2}) c_m^\dagger c_{-m}^\dagger |-\rangle \ . \end{aligned}$$

It can be easily checked that taking $A_{-m2} = A_{m1}$ and $A_{m2} = -A_{-m1}$ for all $m > 0$ makes the above two states identical (up to normalization). The intrinsic Slater determinant $a_1^\dagger a_2^\dagger |-\rangle$ is triaxial; thus we see that projecting a triaxial intrinsic state on $J_z = 0$ can in principle produce an eigenstate of the pairing Hamiltonian. With an increase in the number of particles the situation gets much more complicated. We have examined numerically the case of $j = \frac{15}{2}$ with up to eight particles and have found that in all cases axial-symmetry-projected general Slater determinants provide a very good approximations to the exact eigenstates, in fact always better than those of the conventional BCS approach. Recently a shell-model diagonalization of a pure pairing force in the fp shell has been found to produce triaxial states too [16]. This all seems to indicate that there is a subtle connection between "deformation" in gauge space (particle number violation) and deformation in the usual sense, which certainly calls for a better understanding.

Coming back to our variational procedure, we should not fail to mention its shortcomings. The most serious is that it is not justified for certain many-body states. As an example, consider the lowest $\frac{1}{2}^+$ state of ^{21}Ne. If

we vary the intrinsic states after projecting on $J_z = \frac{1}{2}$, we end up approximating the $J_z = \frac{1}{2}$ component of its $\frac{3}{2}^+$ ground state rather than its $\frac{1}{2}^+$ state. Introducing the approximate full angular momentum projection before variation ($\lambda \neq 0$) slightly improves the situation, but in general we do not recommend the application of our procedure to states that are higher in energy than states of higher spin and with all the same other quantum numbers, since in such cases the quality of the approximation is rather poor.

The results of these first applications of the hybrid-symmetry-conserving variational procedure are very encouraging. Leaving the selection of the relevant configurations to the dynamics of the many-body system allows one to describe its states in terms of a small number of angular-momentum-projected general deformed Slater determinants. The ability of the method to deal with even-even as well as with odd-mass nuclei should make it, despite the limitation discussed above, an extremely useful tool in addressing important nuclear structure questions, often of relevance to other fields (see, e.g., [17]).

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