Many-body approximations in the *sd*-shell "sandbox"

R. A. Sen'kov,[1,2] G. F. Bertsch,[3] B. A. Brown,[1] Y. L. Luo,[3] and V. G. Zelevinsky[1]

[1]*National Superconducting Cyclotron Laboratory and Department of Physics and Astronomy, Michigan State University, East Lansing, Michigan 48824-1321, USA*

[2]*Department of Physics, Novosibirsk State University, Novosibirsk RU-630090, Russia*

[3]*Department of Physics and Institute of Nuclear Theory, Box 351560, University of Washington, Seattle, Washington 98915, USA*

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A new theoretical approach is presented that combines the Hartree-Fock variational scheme with the exact solution of the pairing problem in the finite orbital space. Using this formulation in the *sd*-space as an example, we show that the exact pairing significantly improves the results for the ground state energy.

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I. INTRODUCTION

The classical Hartree-Fock (HF) approximation is a prototype of the modern approach to the quantum many-body problem related to the energy density functional [1,2]. When applied to complex nuclei, the density functional theory may provide a universal description across the nuclear chart. The pairing interaction that is present in nuclei as well as in fermionic condensed matter systems is usually included in the Hartree-Fock-Bogoliubov (HFB) form [3]. The well-known deficiencies of the HFB approach for mesoscopic systems follow mainly from its nonconservation of particle number. As a result, unphysical features are introduced into dynamics, the superfluid phase transition appears too sharp, and the correlational energy produced by pairing might be severely underestimated. As was shown earlier [4,5], the pairing part of the problem can be solved numerically quite easily with the help of the seniority representation in a spherical basis, and its exact solution significantly improves the results. For example, differences between the exact solution of the pairing problem and the BCS theory of up to 2 MeV are found for the Ca isotopes [4].

It was also sketched in Ref. [4] how other parts of the interaction can be incorporated into the exact pairing method in the approximate way that reminds the HF approach. This can be done in an iterative fashion: the exact pairing solution using the starting single-particle basis determines the actual occupation numbers; these (in general, fractional) occupancies self-consistently determine, in the HF spirit, an improved single-particle basis where we again solve the pairing problem, etc., until convergence. In this way both mean-field features, deformation and pairing, can be accounted for. The main purpose of the current work is to further develop this Hartree-Fock plus pairing correlation (HFP) method that essentially is an intermediate step from the HF approach toward the full shell-model (SM) description. On one hand, we would want to keep the simplicity and modest computer demands as inherent properties of the mean-field approach. On the other hand, we take into consideration pairing and other physical effects beyond the simple HF, or mean field in general. We check our approach for the *sd*-shell nuclei, where the SM with large-scale diagonalization works perfectly [6] and can serve as a searchlight illuminating the correct direction of motion. The success of this attempt will allow the extension of the approach to heavy nuclei, where the catastrophic growth of dimensions makes the complete shell-model solution unrealistic.

The main direction of our approach can be historically traced back to the old ideas of constructing the nuclear many-body wave function using the correlated pairs as building blocks. Along these lines one can recall the boson expansion techniques [7,8] (for the latest review and further references see Ref. [9]), interacting boson model [10], nucleon-pair shell model [11], and many other attempts. Our emphasis is quite different however. We consider as the fundamental basis the Hartree-Fock theory and its inherent mean-field concept, and we attempt here to introduce correlations using modern shell-model capabilities.

II. OUTLINE OF THE METHOD

In the spirit of most mean-field approaches, we formulate this method as a variational one. As in the shell model, we assume a general form of the two-body Hamiltonian that includes the single-particle term t and the (antisymmetrized) two-body interaction V:

$$\hat{H} = \sum_{ik} t_{ik} a_i^\dagger a_k + \frac{1}{4} \sum_{ijkl} V_{ijkl} a_i^\dagger a_j^\dagger a_k a_l. \tag{1}$$

The variational wave function $|\Psi\rangle$ is defined below. The wave function and all properties of the system follow from the minimization of the expectation value

$$\langle \Psi | \hat{H} | \Psi \rangle. \tag{2}$$

For our test of the methods, we take for V the USDB interaction from the *sd*-shell model [6]. It allows us to compare the results obtained using our approximate method with the exact shell-model calculations in the same single-particle model space.

The ground state wave function $|\Psi\rangle$ for a fixed particle number N can be presented as a superposition of basis states,

$$|\Psi\rangle = \sum_{d \in D} C_d |d\rangle, \tag{3}$$

where each basis state $|d\rangle$ is a Slater determinant, which for N fermions can be written as usual:

$$|d\rangle = a^\dagger_{\nu_1} a^\dagger_{\nu_2} \cdots a^\dagger_{\nu_N} |0\rangle. \tag{4}$$

The single-particle states ϕ_ν can be found with the help of the variational principle as it is usually done in the HF method. The approach is actually defined by the selection of the space D spanned by the determinants $|d\rangle$. If we choose only one Slater determinant as our variational wave function (3), we come to the standard HF approximation. If the manifold D includes all possible configurations, then we get the exact shell-model solution.

In this article our choice is determined by the pairing phenomenon that smears the Fermi surface and converts the Fermi-gas ground state into a superposition of Slater determinants. In the case of a *spherical* system with the pairing forces taken as the $J = 0, T = 1$ part of the two-body interaction (1), we have seniority s as a good quantum number. For an even number of particles, the ground state has $s = 0$, while for an odd number $s = 1$. In the even spherical case we can construct the basis of Slater determinants $|d\rangle$ occupying single-particle levels $|jm\rangle$ by pairs,

$$\prod_{j;m>0} a^\dagger_{jm} a^\dagger_{j\tilde{m}} |0\rangle, \tag{5}$$

where $a^\dagger_{j\tilde{m}} = (-1)^{j-m} a^\dagger_{j-m}$ is the creation operator for the time-conjugate single-particle state with respect to $a^\dagger_{jm}$. The number of terms in the product in Eq. (5) is determined by the given number of particles. Here we omit all quantum numbers except total angular momentum j and its projection m.

The interaction of neutrons and protons through the mean field does not affect the dimensionalities, but can break spherical symmetry and bring in *deformed* mean fields. In the case of a deformed nucleus, even if we had only the $J = 0$ part of the two-body interaction (1) in the spherical representation, we have to take into consideration a broader class of pairs arising as a result of splitting and mixing of the original spherical states by deformation. Here we limit ourselves by the case of axially symmetric deformation, when the single-particle orbitals $|\nu m\rangle$ are still characterized by the angular momentum projection m along with other quantum numbers ν.

For an even particle number we construct the "paired" basis Slater determinants of the form

$$\prod_{\nu,\kappa;m>0} a^\dagger_{\nu m} a^\dagger_{\kappa -m} |0\rangle. \tag{6}$$

Using this form we hope to correctly account for pairing correlations in the deformed basis. The dimension of this space D is much reduced in comparison with the full shell model. For an odd particle number, we use the same Eq. (6) but add one additional creation operator that corresponds to the odd particle. The odd particle can be placed in any empty single-particle state, and the states are divided into classes with a definite value of the angular momentum projection.

We can restrict the class of states in Eq. (6) further if we consider time-reversal invariance in the density. For an even particle number the basis states then take the form

$$\prod_{\nu;m>0} a^\dagger_{\nu m} a^\dagger_{\nu -m} |0\rangle. \tag{7}$$

For an odd particle number, the density ρ with one additional particle and the Hamiltonian, see below Eq. (10), already are not time-reversal invariant. This means that for each single-particle state we cannot find the exact time-reversal partner. However, the violation of time-reversal invariance due to the odd particle is not very large and we may use the space (7) with one additional particle as an approximation.

The variation over amplitudes C_d with the additional normalization condition of the wave function, $\langle\Psi|\Psi\rangle = 1$, leads us to the usual set of equations,

$$\sum_{d'} \langle d|\hat{H}|d'\rangle C_{d'} = EC_d. \tag{8}$$

The matrix elements $\langle d|\hat{H}|d'\rangle$ are calculated for the determinants built on a given single-particle basis, and Eqs. (8) are solved numerically. The mean-field basis is found from the self-consistent HF equation

$$h(\rho)\phi_\nu = \epsilon_\nu \phi_\nu, \tag{9}$$

where

$$h(\rho) = t + V(\rho) \tag{10}$$

is the single-particle HF Hamiltonian, ϵ_ν are the single-particle energies, and ρ is the density matrix self-consistently determined by

$$\rho_{ij} = \langle\Psi|a^\dagger_j a_i|\Psi\rangle. \tag{11}$$

The mean-field potential is given by its matrix elements,

$$V_{ij}(\rho) = \sum_{kl} V_{iklj}\rho_{lk}. \tag{12}$$

In this conventional mean-field formulation, the potential (12) contains the direct and exchange contributions. The pairing effects, with strict particle number conservation, are contained in the superposition of the Slater determinants (3) used instead of the single HF determinant.

The HFP scheme of solution is the following:

(i) Start with the spherical single-particle basis $|jm\rangle$.
(ii) Choose in this basis the initial diagonal density matrix ρ corresponding to occupation numbers specific for prolate or oblate shapes (pairs with small or large $|m|$, respectively).
(iii) Solve the HF variational Eq. (9) and get the single-particle spectrum (ϕ_ν, ϵ_ν), in general corresponding to a deformed field.
(iv) Construct the "paired" class of many-body basis wave functions according to Eq. (6) and calculate the matrix elements of the Hamiltonian H.
(v) Solve the variational Eq. (8) and obtain the ground state wave function.
(vi) Calculate the next-step density matrix (11).
(vii) Repeat the procedure starting from Step 3 until convergence.

The converged results will certainly be a local minimum of Eq. (2). Exploration of different starting choices in Step 2 is needed to find a global minimum. In our study here we start with a spherical single-particle basis (because the USDB interaction is so defined) but in principle any convenient axial basis could be used. In the end, the ground state energy can be found as the Hamiltonian expectation value over the resulting ground state wave function $|\Psi\rangle$,

$$E_{\rm HFP} = \langle\Psi|\hat{H}|\Psi\rangle. \tag{13}$$

In the current application of our method we make a simplifying approximation treating protons and neutrons separately. It means that, though we consider the full two-body interaction (1) including the $T_z = 0$ part, the variational function (3) is constructed as the product of proton and neutron parts,

$$|\Psi\rangle = |P\rangle \cdot |N\rangle. \tag{14}$$

Each part of this wave function can be build as a superposition of Slater determinants: $|p\rangle$, $|n\rangle$, which include only one sort of particle and have the same form as in Eq. (6),

$$|P\rangle = \sum_{p\in D_p} C_p|p\rangle, \tag{15}$$

$$|N\rangle = \sum_{n\in D_n} C_n|n\rangle, \tag{16}$$

where D_p and D_n are dimensions of the proton and neutron spaces, respectively.

Thus variation over amplitudes C_p and C_n leads to the two sets of equations - for protons and neutrons separately. These equations have the same structure as Eq. (8). The only difference is that for the protons we use an effective Hamiltonian $\hat{H}_p$ that equals to the total Hamiltonian (1) averaged over the neutron part of the wave function, and similar for the neutrons, $\hat{H}_n$:

$$\hat{H}_p = \langle N|\hat{H}|N\rangle, \;\; \hat{H}_n = \langle P|\hat{H}|P\rangle. \tag{17}$$

Clearly we are losing here the proton-neutron correlations although their mutual contributions to the mean field are fully accounted for. We consider the effect of the $T_z = 0$ part in Sec. IV.

III. RESULTS

We performed calculations of ground state energies for all nuclei within the *sd*-shell region, from ^{17}O to ^{39}Ca. Our results [12] are summarized in Figs. 1–5. In Figs. 1 and 2 we show the energy gain from HFP compared to HF,

$$E_{\rm corr} = E_{\rm HF} - E_{\rm HFP}. \tag{18}$$

Typical values are one to a few MeV. One observes the well-known odd-even staggering that is characteristic of pairing. In the conventional HFB approach, the pairing correlation is zero for many of these nuclei, including cases such as ^{24}O, where the spherical shell gap is too large, and cases such as ^{20}Ne, ^{24}Mg, and ^{28}Si, where the deformed shell gap is too large to support the BCS-type pairing. The HFP method gives some correlation energy for all *sd*-shell nuclei for which there are at least two

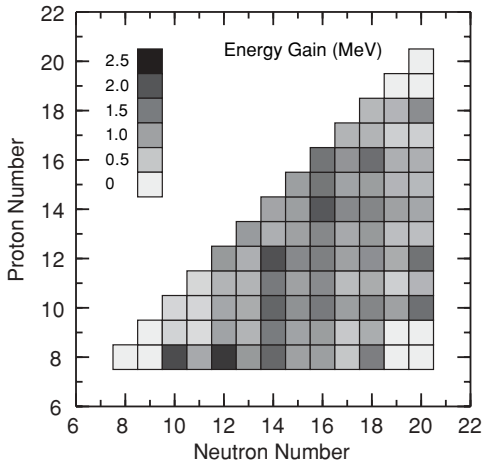

FIG. 1. Pairing correlation energy Eq. (18) for all *sd*-shell nuclei.

active particles ($9 < N < 19$ or $9 < Z < 19$). In the practical solution of the equations we find that many *sd*-shell nuclei have two or three energy minima. To have some confidence that we have found the lowest energy solution we start with several initial values of the density matrix including those that are prolate and oblate deformed, spherical, and random.

In Figs. 3 and 4 we show the difference between the HFP result and the exact shell-model energy both obtained with the USDB Hamiltonian. For comparison of the methods, the full solution for the ground state of ^{28}Si must take into account 93,710 *M*-scheme Slater determinants. When projected onto good $J = 0$ there are 9216 states, and when projected onto good $J = 0, T = 0$ there are 839 states. The HFP method requires 92 determinants for protons and 92 for neutrons.

We have repeated the calculations for all nuclei using the simplified time-reversal basis-state approximation discussed in connection with Eq. (7). This leads to a decrease in the matrix dimension, for example, for ^{28}Si from 92 to 20. The energy difference between the full calculation with Eq. (6) and the reduced calculation with Eq. (7) is 300 keV for ^{28}Si. For all nuclei, typical differences are 100–300 keV with the largest exception being 800 keV for an odd-odd nucleus. The reduction in matrix dimension with the time-reversal

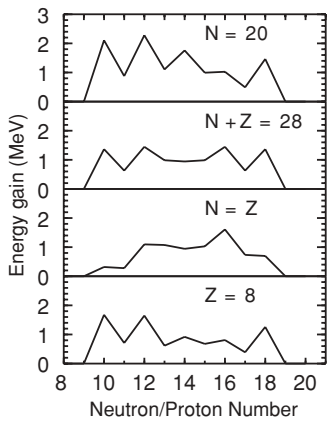

FIG. 2. Four selected cuts on the correlation energies displayed in Fig. 1.

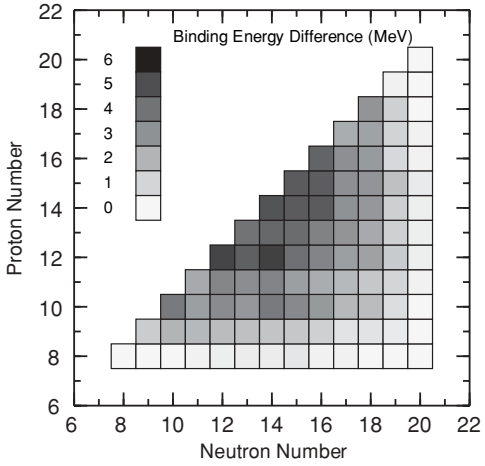

FIG. 3. Energy difference between the exact results and our HFP model for all sd-shell nuclei.

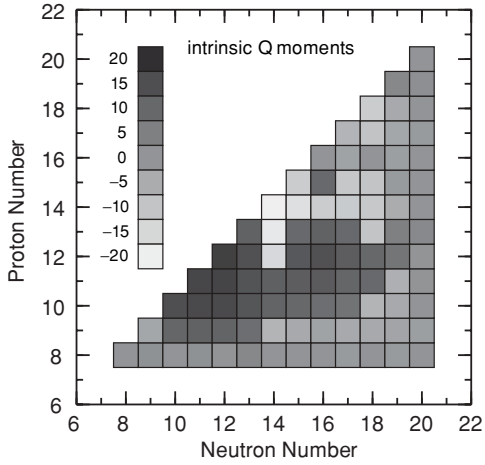

FIG. 5. Intrinsic quadrupole moment Q, in units b^2 (b is the oscillator parameter), for the lowest energy configuration for all sd-shell nuclei.

restriction may be useful when the HFP method is applied to heavy nuclei where the matrix dimensions are of the order of 10,000.

The HFP solution is very close to the exact solution around the edges of the sd-shell (see Fig. 4). These nuclei are spherical and the HFP method is equivalent to the spherical exact-pairing method discussed in Refs. [4] and [5]. The largest deviation from exact is for nuclei near the middle of the sd-shell. There are still pairing contributions for deformed nuclei, but the result is different from the naive expectation of just adding "spherical" contributions. For example, as shown in Fig. 2, the correlation energy is only about 400 keV for the deformed ^{20}Ne, compared to a total of about 3.4 MeV that would be obtained just from adding the 1.7 MeV correlation energies obtained for two neutrons and two protons in a spherical basis (e.g., ^{18}O and ^{18}Ne). But as discussed below in Sec. IV, the pairing correlation contribution to the energies of deformed nuclei with $N = Z$ is increased by the proton-neutron $T = 1$ pairing and by angular-momentum projection.

Finally in Fig. 5 we show the intrinsic quadrupole moment obtained for the lowest energy solutions for all sd-shell nuclei. One observes the well-known region of strongly deformed prolate nuclei near ^{24}Mg. ^{28}Si is the most strongly oblately deformed, and there is an island of weak oblate deformation around ^{31}Si. It would be interesting to use our sd-shell sandbox to clarify the general question of why most nuclei are prolate deformed [13], by exploring the HFP results with different (but realistic) Hamiltonians.

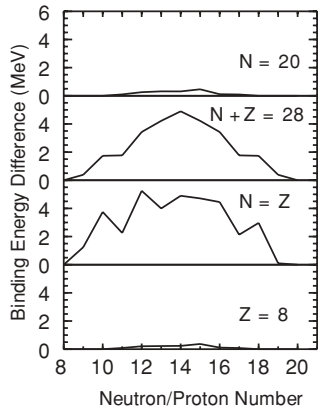

FIG. 4. Four selected cuts on the energy difference between the exact results and our HFP model displayed in Fig. 3.

IV. PROTON-NEUTRON, $T = 1$ PAIRING

The HFP results discussed above contain the pairing correlations due to the neutron-neutron (NN) and proton-proton (PP) two-body interactions. These are the contributions traditionally contained in Hartree-Fock plus pairing models. But for nuclei with $N = Z$ (and those near $N = Z$) one should also include proton-neutron (PN) pairing. To see how this contribution enters we have carried out the full sd-shell calculations in a proton-neutron basis with the USDB Hamiltonian with and without the off-diagonal $J = 0, T = 1$ PN two-body matrix elements. The energy difference between these two calculations is shown in Figs. 6 and 7

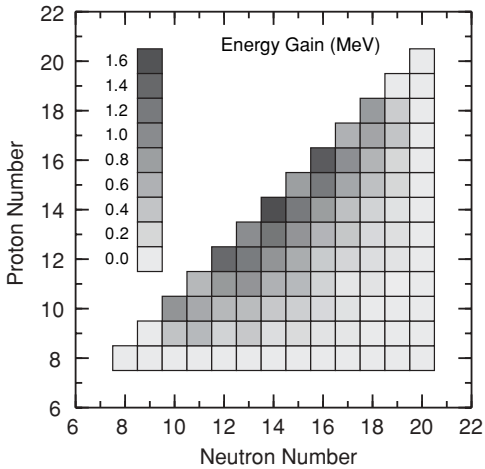

FIG. 6. Energy gain from PN $T = 1$ correlations.

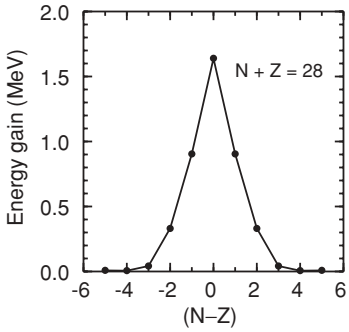

FIG. 7. Energy gain from PN $T = 1$ correlations for $N + Z = 28$.

as the energy gain from PN $T = 1$ pairing. One observes an energy gain strongly peaked at $N = Z$. The dependence on $|N - Z|$ is similar in structure and magnitude to the Wigner term added as corrections to FRDM [14] and HFB [15] fits to nuclear masses. Thus as suggested in Ref. [15], part of the Wigner term can be attributed to PN $T = 1$ pairing. Contributions of the PN $T = 0$ interactions to the Wigner-type mass corrections as discussed in Ref. [16] are also important.

For states with $T = 0$ and $T = 1/2$, isospin symmetry requires that the NN, PP, and PN contributions to $T = 1$ pairing are all equal. Thus it is trivial to add PN pairing to HFP by simply multiplying the PP + NN contribution by 3/2. For higher T there is no exact result, but because the PN pairing contribution is small, it might be approximated or ignored. We note in this context that the PP + NN pairing contribution obtained from the energy gain in HFP over HF (Figs. 1 and 2) for $T = 0$ and $T = 1/2$ is smaller than two times the PN contribution obtained from exact calculations shown in Figs. 6 and 7. This is related to the angular momentum nonconservation in HFP for deformed nuclei. Pairing is reduced in the intrinsic HFP state due to the mixture of higher-J states that have smaller pairing correlations.

V. CONCLUSION

We have extended the exact pairing method developed for spherical nuclei [4,5] to a deformed basis. We have formulated a method called HFP in which the Hamiltonian is diagonalized in a deformed paired basis separately for protons and neutrons. The HFP method gives a pairing correlation energy even in cases where the BCS or HFB approximations would give zero when the energy gap at the Fermi surface is large. In light to medium heavy nuclei HFP can improve the binding energy calculation for a given pairing Hamiltonian by up to 2 MeV. We have also discussed the role of $J = 0$, $T = 1$ pairing between protons and neutrons and have shown that it contributes most strongly to nuclei with $T = 0$ and $T = 1/2$ and contributes to the Wigner term for nuclear binding energy which is often added on an *ad hoc* basis to HF and FRDM models. It can be calculated exactly in HFP for $T = 0$ and $T = 1/2$, can be neglected for $T > 2$, and could be approximated for $T = 1$ and $T = 3/2$.

Obviously, the HFP is still far from adequate away from semi-magic nuclei. The method might be further improved by using the exact but more complicated variational approach relating the single-particle basis to the full set of the coefficients of the superposition (3). The angular momentum nonconservation is certainly a significant deficiency of the wave function that, when repaired, will introduce additional correlation energy. There are a number of ways that rotational correlation energies can be calculated, and we are optimistic that HFP wave functions can be used as a better starting point. Effective Hamiltonians for the HFB solution are explored in Ref. [17]. Finally, some improvement may follow from including the nonaxial configurations with the pairing between more general time-conjugate orbitals (most probably, the mean field in ^{24}Mg is triaxial [18,19]).

ACKNOWLEDGMENTS

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