Isovector and isoscalar proton-neutron pairing in $N > Z$ nuclei

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We propose a particle number conserving formalism for the treatment of isovector-isoscalar pairing in nuclei with $N > Z$. The ground state of the pairing Hamiltonian is described by a quartet condensate to which is appended a pair condensate formed by the neutrons in excess. The quartets are built by two isovector pairs coupled to the total isospin $T = 0$ and two collective isoscalar proton-neutron pairs. To probe this ansatz for the ground state we performed calculations for $N > Z$ nuclei with the valence nucleons moving above the cores ^{16}O, ^{40}Ca, and ^{100}Sn. The calculations are done with two pairing interactions, one state-independent and the other of zero range, which are supposed to scatter pairs in time-reversed orbits. It is proven that the ground-state correlation energies calculated within this approach are very close to the exact results provided by the diagonalization of the pairing Hamiltonian. Based on this formalism we have shown that moving away from the $N = Z$ line, both the isoscalar and the isovector proton-neutron pairing correlations remain significant and that they cannot be treated accurately by models based on a proton-neutron pair condensate.

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I. INTRODUCTION

In spite of many years of theoretical and experimental studies, the role of neutron-proton pairing in nuclei is still a matter of debate (for recent reviews, see Refs. [1,2]). One of the most debated issues is whether in nuclei the isoscalar ($T = 0$) spin-triplet neutron-proton pairs could form a deuteronlike pair condensate and if this condensate would coexist with the condensates of spin-singlet isovector ($T = 1$) pairs [3–7]. Most of the studies have been carried out for heavy nuclei close to the $N = Z$ line in which the spin-triplet pairing is expected to be stronger and less suppressed by the spin-orbit field. Some calculations predict that a spin-triplet phase might exist, alone or mixed with the isovector pairing phase, in the ground state of some nuclei [5,7], but it is not clear yet how much these predictions are affected by the employed approximations. On the experimental side, so far there is no clear evidence for the fingerprints of the proton-neutron pairing phase on measurable quantities [1].

The majority of the theoretical studies mentioned above have been done by treating the pairing in the framework of the generalized Bogoliubov approach, as outlined many years ago by Goodman [8]. This approach is very convenient because it can treat all types of pairing correlations, isovector and isoscalar, on an equal footing. It has, however, the drawback that it does not conserve exactly the particle number and the isospin. An isospin conserving theory can be formulated in terms of alphalike four-body structures (called hereafter alphalike quartets or, simply, quartets) built by coupling two protons and two neutrons to total isospin $T = 0$. One of the first attempts on this line was the treating of the isovector pairing by a BCS-like state based on alphalike quartets [9]. Similar BCS trial states have been employed to study the competition between pairing and quartetting in nuclei [10,11]. Alphalike quartets have been also used to treat pairing in particle number conserving formalisms [12,13]. One of the first such formalisms, employed for the treatment of isovector pairing, was based on quartets built by two neutrons and two protons sitting in the same single-particle orbit [12]. Since this formalism is using noncollective quartets, its application to large systems is cumbersome. An alternative alphalike quartet formalism, based on collective quartets, was proposed in Refs. [14,15]. In this formalism the ground state of isovector paring Hamiltonians is described as a condensate of collective quartets in the case of $N = Z$ nuclei [14], and as a condensate of quartets to which is appended a condensate of neutron pairs in the case of $N > Z$ nuclei [15]. Recently this quartet condensation formalism (QCM) was extended to treat both isovector and isoscalar pairing interactions in $N = Z$ nuclei [16,17]. The scope of this paper is to extend further this approach to $N > Z$ nuclei and to probe the validity of the new approach for isovector and isoscalar pairing Hamiltonians, which can be solved exactly by diagonalization.

II. FORMALISM

Since the present formalism is an extension of the model introduced in Ref. [16], for the sake of completeness we start by briefly presenting this approach. As in Ref. [16], we consider systems formed by neutrons and protons moving in axially deformed mean fields and interacting by isovector and isoscalar pairing forces, which scatter pairs of nucleons in time-reversed single-particle states. These systems are

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described by the Hamiltonian

$$H = \sum_{i,\tau=\pm 1/2} \varepsilon_{i\tau} N_{i\tau} + \sum_{i,j} V_{i,j}^{(T=1)} \sum_{t=-1,0,1} P_{i,t}^{\dagger} P_{j,t} + \sum_{i,j} V_{i,j}^{(T=0)} D_{i,0}^{\dagger} D_{j,0}, \tag{2.1}$$

where $\varepsilon_{i,\tau}$ are single-particle energies associated with the mean field of neutrons ($\tau = 1/2$) and protons ($\tau = -1/2$) while $N_{i,\tau}$ are the particle number operators. The second term is the isovector pairing interaction expressed by the isovector pair operators $P_{i,1}^{\dagger} = \nu_i^{\dagger}\nu_{\bar{i}}^{\dagger}$, $P_{i,-1}^{\dagger} = \pi_i^{\dagger}\pi_{\bar{i}}^{\dagger}$, $P_{i,0}^{\dagger} = (\nu_i^{\dagger}\pi_{\bar{i}}^{\dagger} + \pi_i^{\dagger}\nu_{\bar{i}}^{\dagger})/\sqrt{2}$. The third term is the isoscalar pairing interaction and $D_{i,0}^{\dagger} = (\nu_i^{\dagger}\pi_{\bar{i}}^{\dagger} - \pi_i^{\dagger}\nu_{\bar{i}}^{\dagger})/\sqrt{2}$ is the isoscalar pair operator. By $\nu_i^{\dagger}$ and $\pi_i^{\dagger}$ are denoted the creation operators for neutrons and protons while $\bar{i}$ is the time conjugate of the state i.

It is worth emphasising that the Hamiltonian (1), which is employed in many nuclear structure calculations (e.g., see Ref. [19] and the references quoted therein), describes the correlations associated to the pairs built on time-reversed axially deformed states. As such, these pairs have $J_z = 0$ but not a well-defined angular momentum J. In fact, the isovector and isoscalar pairs with $J_z = 0$ can be written as a particular superposition of pairs with $J = \{0, 2, 4, \ldots\}$ and, respectively, with $J = \{1, 3, 5, \ldots\}$. Therefore the intrinsic Hamiltonian (1) is not physically equivalent with the standard pairing Hamiltonians, which take into account only $J = 0$ and $J = 1$ pairing correlations. By analogy with the $J = 1$ spherically symmetric pairing interactions, in the Hamiltonian (1) one can eventually introduce a more general isoscalar pairing force, which includes also pairs with $J_z = \pm 1$. The role of such pairs in the intrinsic system is an open and interesting question. However, the study of this issue is beyond the scope of this paper.

In most of the studies the Hamiltonian (1) is solved in BCS-like approximations based on the generalized Bogoliubov transformation. An alternative approach, which conserves exactly the particle number and the isospin, was proposed in Ref. [16] for the case of even-even $N = Z$ systems. In this approach, called the quartet condensation model (QCM), the ground state of the Hamiltonian (1) is approximated by the trial state

$$|QCM\rangle = \left(A^{\dagger} + \Delta_0^{\dagger 2}\right)^{n_q}|0\rangle, \tag{2.2}$$

where $n_q = (N + Z)/2$ while $|0\rangle$ is the vacuum state represented by the nucleons, which are supposed to be not affected by the pairing interactions (e.g., an even-even closed core). The operator $A^{\dagger}$ is the isovector quartet built by two isovector noncollective pairs coupled to the total isospin $T = 0$, i.e.,

$$A^{\dagger} = \sum_{i,j} x_{ij} [P_i^{\dagger} P_j^{\dagger}]^{T=0}. \tag{2.3}$$

Assuming that the mixing coefficients are separable, i.e., $x_{ij} = x_i x_j$, the isovector quartet takes the form

$$A^{\dagger} = 2\Gamma_1^{\dagger}\Gamma_{-1}^{\dagger} - (\Gamma_0^{\dagger})^2, \tag{2.4}$$

where

$$\Gamma_t^{\dagger} = \sum_i x_i P_{i,t}^{\dagger} \tag{2.5}$$

are collective pair operators for neutron-neutron pairs ($t = 1$), proton-proton pairs ($t = -1$), and proton-neutron pairs ($t = 0$). The isoscalar degrees of freedom are described by the collective isoscalar pair

$$\Delta_0^{\dagger} = \sum_i y_i D_{i,0}^{\dagger}. \tag{2.6}$$

The trial state (2.2) is called a quartet condensate. The term condensate has here the same meaning as in the case of pair condensate: a state obtained by acting many times with the same operator on a vacuum state.

In what follows we extend this approach to even-even systems with $N > Z$ (the case $N < Z$ is treated in the same manner). As in the QCM approach presented above, by N and Z we denote the numbers of neutrons and protons moving above a self-conjugate core, which plays the role of the reference (vacuum) state. To describe the ground state of the systems with $N > Z$ we use the following ansatz: (i) we assume that the protons together with an equal number of neutrons are forming a four-body condensate with the same structure as in Eq. (2.2); (ii) we assume that the neutrons in excess are forming a pair condensate, which is appended to the four-body condensate. The trial state that corresponds to these assumptions is given by

$$|QCM\rangle = (\tilde{\Gamma}_1^{\dagger})^{n_N}\left(A^{\dagger} + \Delta_0^{\dagger 2}\right)^{n_q}|0\rangle, \tag{2.7}$$

where $n_N = (N - Z)/2$ gives the number of neutron pairs in excess while $n_q = (N + Z - 2n_N)/4$ denotes the maximum number of quartets, which can be formed with Z protons. The extra neutrons are represented by the collective neutron pair

$$\tilde{\Gamma}_1^{\dagger} = \sum_i z_i P_{i,1}^{\dagger}. \tag{2.8}$$

As can be seen, the structure of the extra pairs, expressed by the mixing amplitudes, is different from the structure of the neutron pairs, which enter in the definition of the isovector quartet (2.4). It is worth mentioning that in the particular case when the isoscalar pairs are absent, the state (2.6) is the ansatz employed in Ref. [15] for the description of the ground state of $N > Z$ systems interacting by an isovector pairing interaction.

The state (2.6) has a very complicated structure when it is expressed in terms of pairs. Thus, replacing the quartet operator by (2.4) one can see that the state (2.6) is a superposition of pair condensates, each of them formed by various types of pairs. Among these terms of special interest are the following ones:

$$|C_{iv}\rangle = (\tilde{\Gamma}_1^{\dagger})^{n_N}\left(\Gamma_0^{\dagger 2}\right)^{n_q}|0\rangle, \tag{2.9}$$

$$|C_{is}\rangle = (\tilde{\Gamma}_1^{\dagger})^{n_N}\left(\Delta_0^{\dagger 2}\right)^{n_q}|0\rangle. \tag{2.10}$$

As can be seen, in the first (second) state it is supposed that the proton-neutron correlations are described by a condensate of isovector (isoscalar) proton-neutron pairs. The validity of

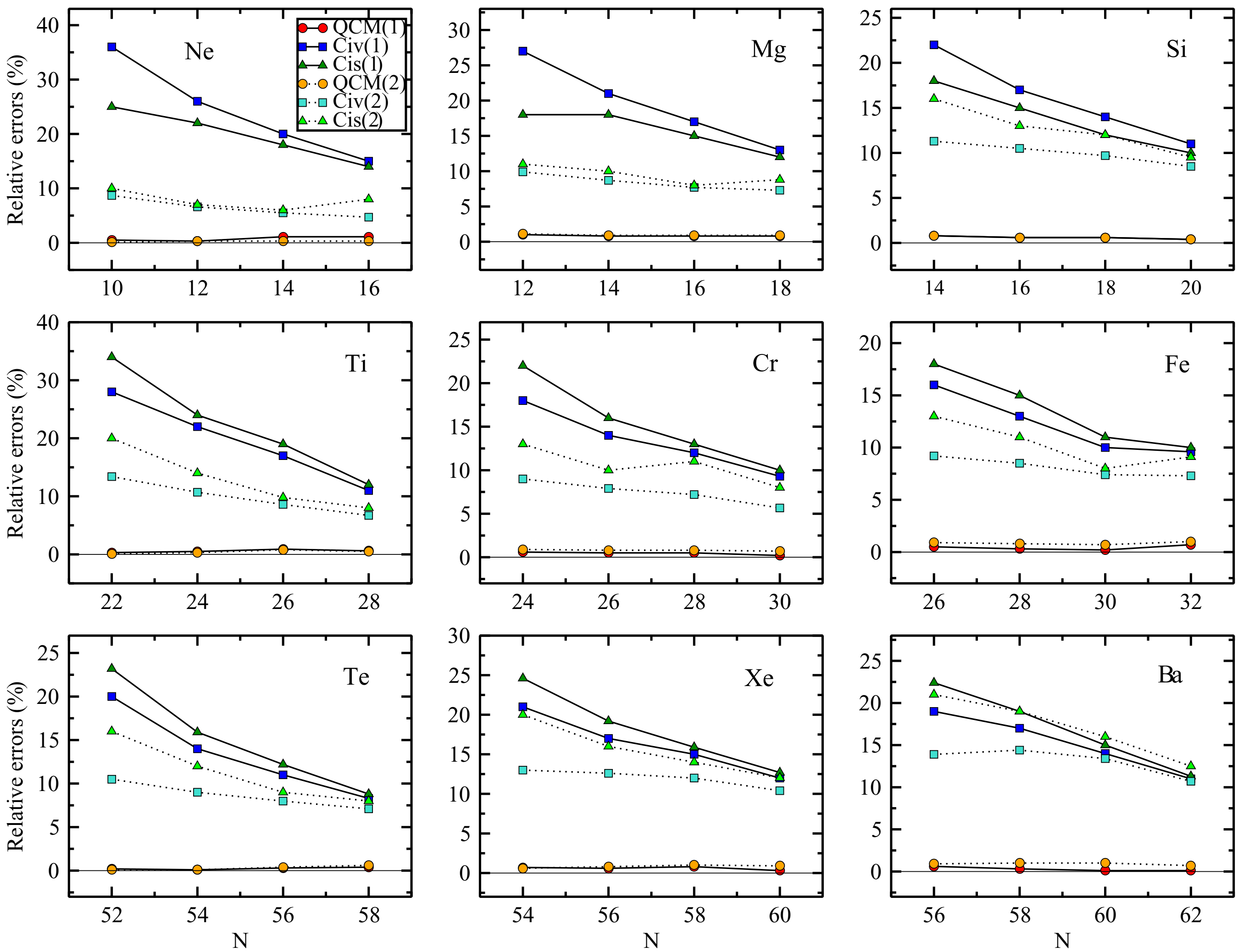

FIG. 1. The errors for the energy correlations as a function of neutron number for various isotopes. The results correspond to the QCM state [Eq. (2.6)] and to the approximations C_{iv} [Eq. (2.8)] and C_{is} [Eq. (2.9)]. The labels 1 and 2 in the brackets refer to the results obtained with the state-independent force and zero-range force, respectively. The errors are calculated relative to the exact results.

these assumptions will be tested below against the full ansatz (2.6).

The trial state (2.6) depends on the mixing amplitudes of the collective pair operators. They are determined variationally by minimizing the average of the Hamiltonian under the normalization condition imposed to the trial state. Details about the calculation scheme are presented in the Appendix.

III. RESULTS

To probe the accuracy of the approach presented above we use the same examples as in Refs. [15,16]. Namely, we consider three sets of nuclei with the valence neutrons and protons moving above the cores ^{16}O, ^{40}Ca, and ^{100}Sn. We start by the even-even $N = Z$ systems obtained by adding to each core one, two, and three quartets, which are described by the trial state (2.2). Then, on the top of these $N = Z$ nuclei we add up to three neutron pairs; these $N > Z$ systems are described by the trial state (2.6). The nucleons are supposed to move in the lowest ten single-particle states above the closed cores mentioned above. These states are generated by axially deformed Skyrme-HF calculations performed for the $N = Z$ nuclei. In the mean-field calculations we have employed the Skyrme functional SLy4 [20] and we have neglected the Coulomb interaction. The deformed mean field in which the nucleons are moving is determined self-consistently by the Skyrme functional, which takes also into account all the degrees of freedom, which are not associated to the pairing channel.

What remains to be chosen are the pairing interactions. How to fix these interactions for nuclei with neutrons and protons in the same valence shell is not clearly established, especially for the case of isoscalar pairing force. The simplest interaction that is usually taken in the isovector pairing channel is a state-independent force. Here we have chosen such an interaction of strength $V_1 = -24/A$, where A is the atomic mass of the nucleus. For the isoscalar interaction we use the same force as in the isovector channel but of different strength, i.e., $V_0 = wV_1$, where w is a scaling factor. For the latter many values have been employed in the literature, ranging

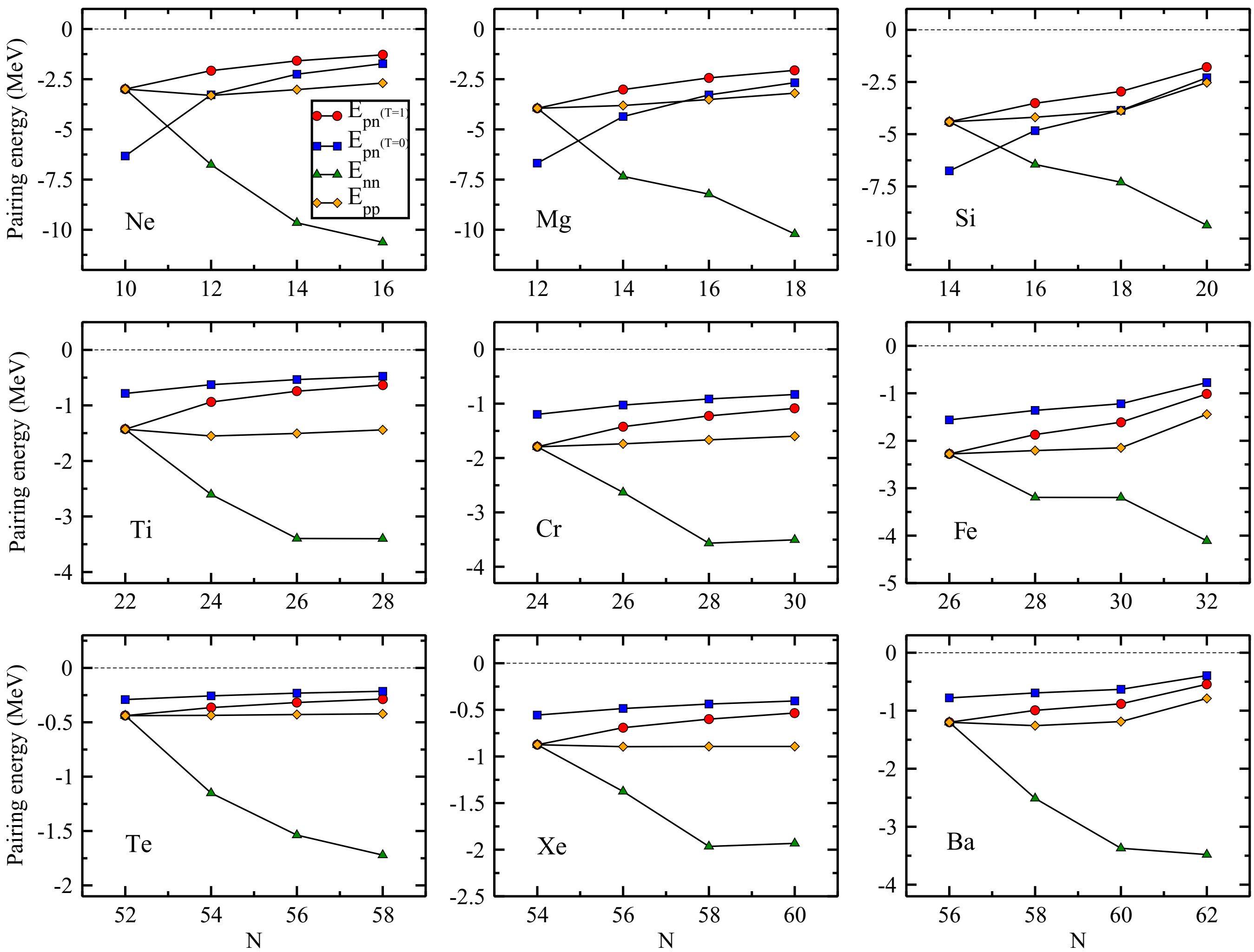

FIG. 2. Pairing energies, defined by Eqs. (3.11)–(3.12), as a function of neutron number, for various nuclei. E_{pn}^{T}, E_{nn}, and E_{pp} denote, respectively, the proton-neutron, neutron-neutron, and proton-proton pairing energies while T is the isospin.

from $w = 1.5$ [2,7] to values smaller than 1 [18]. To cover these situations, here we have chosen two values, $w = 1.2$ and $w = 0.8$. The first value we have employed for sd-shell nuclei and the latter for the heavier nuclei. We have made this choice because it is expected that in pf-shell nuclei the isoscalar pairing interaction is more suppressed than in sd-shell nuclei due to the spin-orbit splitting.

In addition to the state-independent interactions mentioned above, we consider also a zero-range δ interaction $V^T(r_1, r_2) = V_0^T \delta(r_1 - r_2)\hat{P}^T_{S,S_z}$, where $\hat{P}^T_{S,S_z}$ is the projection operator on the spin of the pairs, i.e., $S = 0$ for the isovector ($T = 1$) force and $S = 1$, $S_z = 0$ for the isoscalar ($T = 0$) force. For the strengths V_0^T we have chosen the values employed in Ref. [17], which provide a reasonable description of the lowest $T = 1$ and $T = 0$ states in odd-odd $N = Z$ nuclei. These values are $V_0^{T=1} = 465$ MeV fm^{-3} and $V_0^{T=0} = wV_0^{T=1}$, where $w = 1.6$ for sd-shell nuclei and $w = 1.0$ for the heavier nuclei.

With the two pairing forces we have tested the ansatz (2.6) for the ground-state energy of Hamiltonian (1) considering the $N > Z$ systems mentioned above. To evaluate the accuracy of the approach we have analyzed the ground-state correlation energies defined by $E_{\text{corr}} = E_0 - E$, where E is the ground-state energy and E_0 is the energy in the absence of the interactions. The correlation energies are compared to the exact values obtained by diagonalizing the Hamiltonian (1). The errors, with respect to the exact results, are shown in Fig. 1. One can observe that for all the systems the errors are small, under 1%, which demonstrates that the QCM ansatz (2.6) is describing very well the ground-state pairing correlations. In Fig. 1 are shown also the errors corresponding to the pair condensates given by Eqs. (2.8), (2.9). It can be seen that the errors corresponding to these trial states are much larger. They are the largest for the $N = Z$ nuclei and then they decrease for the systems with extra neutrons. These results indicate that going off the $N = Z$ line there is not a fast transition towards a pure condensate of proton-neutron pairs, of isovector or isoscalar kind.

To illustrate how the pairing correlations are affected by the extra neutrons, in Fig. 2 are plotted, for the state-independent interaction, the average of the isovector and isoscalar pairing forces. The latter are defined by

$$E_t^{(T=1)} = V_1 \sum_{i,j,t} \langle QCM|P_{i,t}^\dagger P_{j,t}|QCM\rangle, \quad (3.11)$$

$$E_{pn}^{(T=0)} = V_0 \sum_{i,j} \langle QCM|D_{i,0}^\dagger D_{j,0}|QCM\rangle. \quad (3.12)$$

The isovector pairing energies corresponding to isospin projections $t = \{1, -1, 0\}$ are denoted by E_{nn}, E_{pp}, and $E_{pn}^{(T=1)}$. As seen in Fig. 2, with the chosen parameters are covered two scenarios concerning the proton-neutron pairing energies, i.e., nuclei with $E_{pn}^{(T=0)} > E_{pn}^{(T=1)}$ and nuclei with $E_{pn}^{(T=0)} < E_{pn}^{(T=1)}$. As expected, the proton-neutron pairing energies are decreasing when extra neutrons are added. For the sd-shell nuclei $E_{pn}^{(T=0)}$ is decreasing faster than $E_{pn}^{(T=1)}$ while for the heavier nuclei the situation is opposite. However, although the proton-neutron energies are decreasing, they remain significantly large, even for the systems with six extra neutrons. Similar features are observed for the zero-range δ interaction. Thus, in variance to the predictions of many BCS-like studies, these calculations show that the isoscalar and isovector proton-neutron pairing correlations: (i) coexist together in both $N = Z$ and $N > Z$ nuclei; (ii) do not vanish quickly by adding few extra neutrons pairs.

IV. SUMMARY

We have discussed the treatment of isovector and isoscalar pairing Hamiltonians for the $N > Z$ systems, with the valence nucleons moving in the same single-particle orbits. The ground state of these pairing Hamiltonians is described by a condensate of quartets to which is appended a condensate built with the neutron pairs in excess. The validity of this ansatz for the ground state was checked for nucleons moving above the cores ^{16}O, ^{40}Ca, and ^{100}Sn, and for two pairing interactions, one state-independent and the other a state-dependent zero-range force. It is shown that the ansatz used for the ground state provides correlation energies which are very close to the results obtained by diagonalizing exactly the pairing Hamiltonian. The present calculations show that the pairing correlations remain significant, in both channels, even in the case when six extra neutrons are added to a $N = Z$ nucleus.

In this paper the extended quartet condensation model (QCM) was applied for a set of nucleons moving in a fixed mean field generated by Skyrme-HF calculations. The same formalism can be employed for performing self-consistent Skyrme-HF + QCM calculations, iterating together the mean-field and the pairing calculations. A similar calculation scheme was applied in Ref. [21] for analyzing the effect of isovector pairing on Wigner energy. The extended QCM formalism presented in this paper is well suited to study how the Wigner energy is affected by both the isovector and the isoscalar pairing correlations. This study is the scope of a future publication.

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APPENDIX

In what follows we present the calculation scheme for evaluating analytically the average of the Hamiltonian $\langle QCM|H|QCM\rangle$ and the norm $\langle QCM|QCM\rangle$. The calculations are performed in the basis spanned by the states

$$|n_1 n_2 n_3 n_4 n_5\rangle = \Gamma_1^{\dagger n_1} \Gamma_{-1}^{\dagger n_2} \Gamma_0^{\dagger n_3} \Delta_0^{\dagger n_4} \tilde{\Gamma}_1^{\dagger n_5} |0\rangle, \quad (A1)$$

where n_i denotes the numbers of collective pairs of a certain type, which can take any value from zero to the maximum number of pairs considered in the pairing Hamiltonian. In this basis the trial state $|QCM\rangle$ [Eq. (2.7)] can be written as

$$|QCM\rangle = \sum_{k_1=0}^{n_q} \sum_{k_2=0}^{n_q-k_1} \binom{k_1}{n_q} \binom{k_2}{n_q - k_1} 2^{n_q-k_1-k_2} (-1)^{k_2} |n_q - k_1 - k_2, n_q - k_1 - k_2, 2k_2, 2k_1, n_N\rangle,$$

where n_q is the number of quartets and n_N is the number of neutron pairs in excess.

To calculate the matrix elements of the Hamiltonian in the basis (1) one needs to evaluate the action of the basic operators $\hat{O} \equiv \{N_{i,\tau}, P_{j,t}, D_{j,0}\}$ on a generic state $|n\rangle \equiv |n_1 n_2 n_3 n_4 n_5\rangle$. To determine these actions we make use of the commutation relation

$$[\hat{O}, G^{\dagger n_i}] = n_i G^{\dagger(n_i-1)} [\hat{O}, G^\dagger] + \frac{n_i(n_i-1)}{2} [[\hat{O}, G^\dagger], G^\dagger] G^{\dagger(n_i-2)}, \quad (A2)$$

where $G^\dagger$ denotes the collective pair operators, which appear in the definition (1). The right-hand side of Eq. (2) involves the commutation relations between the noncollective pair operators and between the latter and the particle number operators, which are provided below.

The commutators between the isovector pair operators are $[P_{k,\pm1}, P_{l,\pm1}^\dagger] = (1 - N_{k,\pm1/2})\delta_{kl}$, $[P_{k,\pm1}, P_{l,\mp1}^\dagger] = 0$, $[P_{k,0}, P_{l,0}^\dagger] = [1 - \frac{1}{2}(N_{k,+1/2} + N_{k,-1/2})]\delta_{kl}$, $[P_{k,0}, P_{l,\pm1}^\dagger] = \pm T_{k,\pm1}\delta_{kl}$, $[P_{k,\pm1}, P_{l,0}^\dagger] = \mp T_{k,\mp1}\delta_{kl}$. The last two commutators generate the isospin operators $T_{k,\pm1}$ defined by $T_{k,1} = -(\nu_i^\dagger \pi_i + \nu_{\bar{i}}^\dagger \pi_{\bar{i}})/\sqrt{2}$ and $T_{k,-1} = +(\pi_i^\dagger \nu_i + \pi_{\bar{i}}^\dagger \nu_{\bar{i}})/\sqrt{2}$.

The commutator between the isoscalar pairs is $[D_{k,0}, D_{l,0}^\dagger] = [1 - \frac{1}{2}(N_{k,+1/2} + N_{k,-1/2})]\delta_{kl}$. The commutators between isovector and isoscalar pair operators are: $[P_{k,p}, D_{l,0}^\dagger] = (-1)^{p+1} W_{k,0,-p}\delta_{kl}$ and $[D_{k,0}, P_{l,p}^\dagger] = -W_{k,0,p}\delta_{kl}$. In these expressions the W operators are given by $W_{k,0,+1} = (-\nu_i^\dagger \pi_i + \nu_{\bar{i}}^\dagger \pi_{\bar{i}})/\sqrt{2}$, $W_{k,0,-1} = (\pi_i^\dagger \nu_i - \pi_{\bar{i}}^\dagger \nu_{\bar{i}})/\sqrt{2}$, and $W_{k,0,0} = (\nu_i^\dagger \nu_i - \pi_i^\dagger \pi_i - \nu_{\bar{i}}^\dagger \nu_{\bar{i}} + \pi_{\bar{i}}^\dagger \pi_{\bar{i}})/2$.

In order to close the commutator algebra, one needs also the commutators involving the particle number, the isospin and the W operators. These commutators are $[N_{k,\pm1/2}, P_{l,p}^\dagger] =$

$(1 \pm p)P^{\dagger}_{l,p}\delta_{kl}$, $[N_{k,\pm 1/2}, D^{\dagger}_{l,0}] = D^{\dagger}_{l,0}\delta_{kl}$; $[T_{k,p}, P^{\dagger}_{l,p'}] = 0$, for $p = p'$, $[T_{k,1}, P^{\dagger}_{l,-1}] = -P^{\dagger}_{k,0}\delta_{kl}$, $[T_{k,-1}, P^{\dagger}_{l,1}] = P^{\dagger}_{k,0}\delta_{kl}$, $[T_{k,\pm 1}, P^{\dagger}_{l,0}] = \mp 1 P^{\dagger}_{\pm 1}\delta_{kl}$, $[T_{k,\pm 1}, D^{\dagger}_{l,0}] = 0$; $[W_{k,0,p}, P^{\dagger}_{l,p'}] = (-1)^p D^{\dagger}_{k,0}\delta_{p,-p'}\delta_{kl}$, and $[W_{k,0,p}, D^{\dagger}_{l,0}] = P^{\dagger}_{k,p}\delta_{kl}$.

With the relation (2) and the commutators listed above one can calculate the action of the basic operators of the Hamiltonian on the basis states (1). As an example we present here the expression corresponding to the action of the pair operator $P_{j,1}$:

$$\begin{aligned} P_{j,1}|n\rangle = & -2n_1n_5x_jz_jP^{\dagger}_{j,1}|n_1-1n_2n_3n_4n_5-1\rangle - n_1(n_1-1)x_j^2P^{\dagger}_{j,1}|n_1-2n_2n_3n_4n_5\rangle \\ & - n_5(n_5-1)z_j^2P^{\dagger}_{j,1}|n_1n_2n_3n_4n_5-2\rangle - \frac{n_3(n_3-1)}{2}x_j^2P^{\dagger}_{j,-1}|n_1n_2n_3-2n_4n_5\rangle \\ & + \frac{n_4(n_4-1)}{2}y_j^2P^{\dagger}_{j,-1}|n_1n_2n_3n_4-2n_5\rangle - n_1n_3x_j^2P^{\dagger}_{j,0}|n_1-1n_2n_3-1n_4n_5\rangle \\ & - n_3n_5x_jz_jP^{\dagger}_{j,0}|n_1n_2n_3-1n_4n_5-1\rangle - n_4n_5y_jz_jD^{\dagger}_{j,0}|n_1n_2n_3n_4-1n_5-1\rangle \\ & - n_1n_4x_jy_jD^{\dagger}_{j,0}|n_1-1n_2n_3n_4-1n_5\rangle + n_1x_j|n_1-1n_2n_3n_4n_5\rangle + n_5z_j|n_1n_2n_3n_4n_5-1\rangle. \end{aligned}$$

The expression above can be then employed to calculate the matrix elements of the two-body operator $\langle m|P^{\dagger}_{i,1}P_{j,1}|n\rangle[=(P_{i,1}|m\rangle)^{\dagger}\times(P_{j,1}|n\rangle)]$. These matrix elements depend recursively on the matrix elements of the basic operators, $P_{i,t}$ and $D_{i,0}$, and on the matrix elements of the two-body operators $P^{\dagger}_{i,t}P_{j,t'}$, $D^{\dagger}_{i,0}D_{j,0}$, and $P^{\dagger}_{i,t}D_{j,0}$. For all these matrix elements one needs to derive the corresponding recurrence relations, which are all coupled together. In addition, these matrix elements depend on the overlaps between auxiliary states, which can be expressed in terms of the matrix elements of the pair operators. For example, $\langle m|n\rangle = \sum_i x_i\langle n_1-1n_2n_3n_4n_5|P_{i,1}|m\rangle$.

Employing the calculations scheme presented above one can derive all the recurrence relations needed to calculate the average of the Hamiltonian. This average is a function of the amplitudes x_i, y_i, z_i, which define the collective pair operators. These amplitudes are determined from the minimization of the average of the Hamiltonian under the constraint $\langle QCM|QCM\rangle = 1$. The variational calculations are done using a minimization subroutine from NAG/LIB. In order to check and to fasten the numerical calculations, for the systems treated in this paper we have also derived analytically the average of the Hamiltonian by employing the symbolic computer algebra system CADABRA (https://cadabra.science/).

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