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Proton–neutron pairing in $N = Z$ nuclei: Quartetting versus pair condensation

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A B S T R A C T

The isoscalar proton–neutron pairing and isovector pairing, including both isovector proton–neutron pairing and like-particle pairing, are treated in a formalism which conserves exactly the particle number and the isospin. The formalism is designed for self-conjugate ($N = Z$) systems of nucleons moving in axially deformed mean fields and interacting through the most general isovector and isoscalar pairing interactions. The ground state of these systems is described by a superposition of two types of condensates, i.e., condensates of isovector quartets, built by two isovector pairs coupled to the total isospin $T = 0$, and condensates of isoscalar proton–neutron pairs. The comparison with the exact solutions of realistic isovector–isoscalar pairing Hamiltonians shows that this ansatz for the ground state is able to describe with high precision the pairing correlation energies. It is also shown that, at variance with the majority of Hartree–Fock–Bogoliubov calculations, in the present formalism the isovector and isoscalar pairing correlations coexist for any pairing interactions. The competition between the isovector and isoscalar proton–neutron pairing correlations is studied for $N = Z$ nuclei with the valence nucleons moving in the *sd* and *pf* shells and in the major shell above ^{100}Sn. We find that in these nuclei the isovector pairing prevail over the isoscalar pairing, especially for heavier nuclei.

1. Introduction

Many nuclei develop correlations among the valence nucleons which can be treated approximatively as a BCS condensate of Cooper pairs [1]. This approximation works reasonably well for heavy nuclei with neutrons and protons moving in different major shells, in which the like-particle pairing plays the dominant role. However, in spite of many years of studies, it is not clear yet which are the physically relevant correlations induced by the pairing interactions in nuclei with $N \approx Z$. In particular, the most debated issues are: (i) whether in $N = Z$ nuclei the pairing can generate a condensate of isoscalar proton–neutron pairs; (ii) if this pairing phase would coexist with the condensate of isovector proton–neutron pairs and like-particle pairs; (iii) what could be the fingerprints of a condensate of isoscalar proton–neutron pairs in the experimental data (for a recent overview on proton–neutron pairing in nuclei see [2]). From theoretical point of view the first two issues have been studied mainly in the framework of Hartree–Fock–Bogoliubov (HFB) approach, which has the advantage of providing an unitary treatment of like-particle and proton–neutron pairing, both isovector and isoscalar (e.g., see [3,4] and the references quoted therein). These studies show that: (a) in most of the cases the isovector and isoscalar proton–neutron pairing correlations do not coexist; (b) the type of pairing which prevails depends strongly on the relative strength of isovector and isoscalar pairing forces.

In the HFB calculations the particle number and the isospin are not conserved exactly, a drawback which could affect significantly the competition between $T = 0$ and $T = 1$ proton–neutron pairing (e.g., see [5]). Exactly solvable models in which the particle number and the isospin are conserved [6–10] show that in fact the fundamental ansatz of the HFB theory, which assumes that the ground state of nuclei can be described by a condensate of Cooper pairs, is not appropriate for $N = Z$ systems. Thus, the SO(5) model for isovector pairing interaction shows that in the case of degenerate levels the ground state of $N = Z$ systems is described by a condensate of quartets [6] and not by a condensate of Cooper pairs, as assumed by the BCS-type approximations. In Refs. [11] it was demonstrated that this is actually the case not only for the schematic SO(5) model but also for any realistic isovector pairing

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Hamiltonian. More precisely, it has been shown that: (i) a condensate of collective quartets, built by two isovector pairs coupled to total isospin $T = 0$, describes the pairing correlation energies of $N = Z$ nuclei with a very good precision (errors under 1%); (ii) in nuclei with $N > Z$ the isovector pairing correlations are accurately described by a quartet condensate to which it is appended a pair condensate formed by the neutron pairs in excess [12]; (iii) the isovector pairing, when treated by the quartet condensation formalism, is able to describe reasonably well the Wigner energies in $N \approx Z$ nuclei [13].

In this Letter we extend the quartet formalism of Ref. [11] for treating both the isovector and the isoscalar pairing interactions. The formalism proposed here is dedicated to those isovector and isoscalar pairing interactions which scatter pairs of nucleons in time-reversed states of axially-deformed mean fields. These are the pairing interactions which are commonly employed in many nuclear structure calculations, e.g., the ones related to beta decays studies [14].

2. Formalism

The systems investigated here are composed of an equal number of neutrons and protons which move in a deformed mean field with axial symmetry. The nucleons are interacting through an isoscalar proton–neutron pairing force and an isovector pairing force, the latter including the proton–neutron pairing and like-particle pairing. The Hamiltonian which describes these systems is given by:

$$\hat{H} = \sum_{i,\tau=\pm 1/2} \varepsilon_{i\tau} N_{i\tau} + \sum_{i,j} V^{T=1}(i,j) \sum_{t=-1,0,1} P^+_{i,t} P_{j,t} + \sum_{i,j} V^{T=0}(i,j) D^+_{i,0} D_{j,0}, \tag{1}$$

where $\varepsilon_{i\tau}$ are the single-particle energies associated to the mean fields of neutrons ($\tau = 1/2$) and protons ($\tau = -1/2$). In the case of axially-deformed mean fields, supposed here, the single-particle states are labeled by $i = \{a, \Omega\}$, where Ω is the projection of the angular momentum on z-axis and a denotes the other quantum numbers which specify the states. The second term is the most general isovector pairing interaction expressed by the non-collective pair operators $P^+_{i,1} = \nu^+_i \nu^+_{\bar{i}}$, $P^+_{i,-1} = \pi^+_i \pi^+_{\bar{i}}$ and $P^+_{i,0} = (\nu^+_i \pi^+_{\bar{i}} + \pi^+_i \nu^+_{\bar{i}})/\sqrt{2}$. The third term is the isoscalar proton–neutron pairing interaction and $D^+_{i,0} = (\nu^+_i \pi^+_{\bar{i}} - \pi^+_i \nu^+_{\bar{i}})/\sqrt{2}$ is the operator which creates a non-collective isoscalar proton–neutron pair. The operators ν^+_i and π^+_i create, respectively, a neutron and a proton in the state i while $\bar{i} = \{a, -\Omega\}$ denotes the time conjugate of the state i.

It can be observed that all pairs operators considered above are constructed with the nucleons in time-reversed and axially-deformed states. Therefore the pairs have $J_z = 0$, where J_z is the projection of the angular momentum on z-axis, but not a well-defined J. In fact, the isovector pairs and the isoscalar pairs with $J_z = 0$, built with axially deformed states, can be seen as a superposition of pairs with $J = \{0, 2, 4, ..\}$ and, respectively, $J = \{1, 3, 5, ..\}$. Therefore the Hamiltonian (1) is not physically equivalent with the spherically-symmetric pairing Hamiltonians in which are taken into account only $J = 0$ isovector pairs and $J = 1$ isoscalar proton–neutron pairs. For the latter case a quartet-type formalism, different from the one presented below, has been proposed in Ref. [15].

The Hamiltonian (1) has been employed, with various single-particle energies and pairing interactions, in many studies. In most of them the Hamiltonian (1) was treated in HFB approximation in which, through a general Bogoliubov transformation, the protons and neutrons are mixed together to form generalized quasiparticles. As a consequence, in HFB the particle number and the isospin are not conserved. Here we present a different approach in which both quantities are conserved exactly from the outset through the way in which the trial wave function is constructed.

As in Ref. [11], for describing the isovector pairing correlations we use as building blocks collective isovector quartets formed by two isovector pairs coupled to the total isospin $T = 0$, i.e.,

$$A^+ = \sum_{i,j} \bar{x}_{ij} [P^+_i P^+_j]^{T=0} = \sum_{ij} x_{ij} (P^+_{i,1} P^+_{j,-1} + P^+_{i,-1} P^+_{j,1} - P^+_{i,0} P^+_{j,0}). \tag{2}$$

Supposing that the amplitudes x_{ij} are separable in the indices i and j, the collective quartet operator can be written as

$$A^+ = 2\Gamma^+_1 \Gamma^+_{-1} - (\Gamma^+_0)^2, \tag{3}$$

where $\Gamma^+_t = \sum_i x_i P^+_{i,t}$ denote, for $t = 0, 1, -1$, the collective Cooper pair operators for the proton–neutron, neutron–neutron and proton–proton pairs.

For treating the isoscalar proton–neutron correlations we use the collective isoscalar pairs defined by

$$\Delta^+_0 = \sum_i y_i D^+_{i,0} = \sum_i y_i (\nu^+_i \pi^+_{\bar{i}} - \pi^+_i \nu^+_{\bar{i}})/\sqrt{2}. \tag{4}$$

With the collective quartet (3) and the collective isoscalar proton–neutron pair (4) we construct the following approximation for the ground sate of Hamiltonian (1)

$$|\Psi\rangle = (A^+ + (\Delta^+_0)^2)^{n_q} |0\rangle, \tag{5}$$

where $n_q = (N + Z)/4$ is the number of quartets one can form with the protons and neutrons ($N = Z$) participating to the pairing correlations.

The ansatz (5) for the ground state is suggested by the exact solution of Hamiltonian (1) for a set of degenerate states and for pairing forces of equal strength, i.e., $g = V^{T=1}(i,j) = V^{T=0}(i,j)$. We have found that in this case the state (5) is the exact ground state of the Hamiltonian (1). The exact ground state energy, when the single-particle energies are put to zero, is given by

$$E(n_q, \nu) = 2gn_q(\nu - n_q + b), \tag{6}$$

where n_q is the number of quartets, ν is the number of double-degenerate single-particle levels and $b = 2$. It should be noticed that this particular solution is not the one corresponding to the isovector–isoscalar pairing Hamiltonian with SU(4) symmetry [6]. In the latter case the isoscalar proton–neutron interaction acts in three channels $\{S = 1, S_z = -1, 0, 1\}$ while here we consider only the isoscalar proton–neutron pairs in time-reversed states.

It can be seen that the state (5) is a superposition of terms formed by a product of quartet condensates and condensates of isoscalar pairs. In particular, it contains two terms, one formed by a quartet condensate and the other by a condensate of isoscalar pairs. They are denoted by:

$$|iv\rangle = (A^+)^{n_q} |0\rangle, \tag{7}$$

$$|is\rangle = (\Delta^+_0)^{2n_q} |0\rangle. \tag{8}$$

The quartet condensate (7) is the ansatz used in Refs. [11] to describe the isovector pairing correlations in the ground state of $N = Z$ nuclei. From Eq. (3) one can see that the quartet condensate

(7) is in fact a superposition of like-particle and proton–neutron pair condensates.

It is worth mentioning that the state (7) is not a boson condensate since the quartet (2) is not a boson operator. Following Ref. [6], we call the state (7) a quartet condensate in order to indicate that it is composed by identical quartets, i.e., quartets described by the same wave function. Therefore here quartet condensation has a similar meaning to the Cooper pair condensation in BCS-like models.

The state (8) is a projected-BCS (PBCS) state, similar to the PBCS states employed for treating the like-particle pairing. The states (7) and (8) are the exact solutions of the isovector and, respectively, the isoscalar pairing interactions of the Hamiltonian (1) for the case of degenerate states. The exact eigenvalues are given by Eq. (6) with $b = 3/2$ for isovector pairing and $b = 1/2$ for isoscalar pairing. It is interesting to observe that Eq. (6) is in all pairing channels similar to the exact solution of the seniority model for like-particle pairing (e.g., see [16]), the only difference appearing in the value of the quantity b.

The state (5) depends on the parameters x_i and y_i which define the collectivity of isovector and isoscalar pairs. They are determined variationally from the minimization of the average of the Hamiltonian and from the condition of normalization of the state (5). To calculate the average of the Hamiltonian on the trial state (5), preserving the Pauli principle exactly, is not a trivial task. In order to evaluate analytically the average of the Hamiltonian and the norm we use the auxiliary states

$$|n_1 n_2 n_3 m\rangle = \Gamma_1^{+n_1}\Gamma_{-1}^{+n_2}\Gamma_0^{+n_3}\Delta_0^{+m}|0\rangle \tag{9}$$

and the recurrence relations method of Ref. [11]. The details of the calculation method, which involves long expressions, are presented in Ref. [17].

3. Results and discussions

One of the most important property of the present formalism for isovector–isoscalar pairing is the prediction that all types of pairing correlations coexist for any pairing interactions. In order to illustrate that, we consider a system formed by four proton–neutron pairs moving in 10 equidistant levels and interacting through state-independent isovector and isoscalar interactions with the strengths given, respectively, by $g_1 = g(1-x)/2$ and $g_0 = g(1+x)/2$. For the strength g we take the value 0.6 (in units of the levels spacing) while the parameter x is varied between -1 and 1. In Fig. 1 we show how the isovector and isoscalar proton–neutron pairing energies are evolving when one goes from an isovector pairing force to an isoscalar pairing force. The proton–neutron pairing energies are defined as the averages $E_{pn}^{T=1} = \langle\Psi|g_1\sum_{i,j}P_{i,0}^{+}P_{j,0}|\Psi\rangle$ and $E_{pn}^{T=0} = \langle\Psi|g_0\sum_{i,j}D_{i,0}^{+}D_{j,0}|\Psi\rangle$. We observe that the predictions of the present formalism, called hereafter the pair-quartet condensation model (PQCM), follows very closely the exact pairing energies (shown by dashed lines) obtained by diagonalization. In order to evidence how evolve the two types of pairing correlations with the pairing forces, in Fig. 1 we display the overlaps between the ground state (5) and the two terms of it defined by the quartet condensate (7) and the condensate of isoscalar pairs (8). These overlaps show a smooth transition from a condensate of quartets to a condensate of pairs, the two types of correlations coexisting in the ground state for any ratio between the strengths of the two pairing forces. It is worth noticing however that the relation of these overlaps to the amount of isovector and isoscalar pairing correlations in the ground state is not straightforward because the state (5) contains, besides the states (7) and (8), a third component formed by the product of

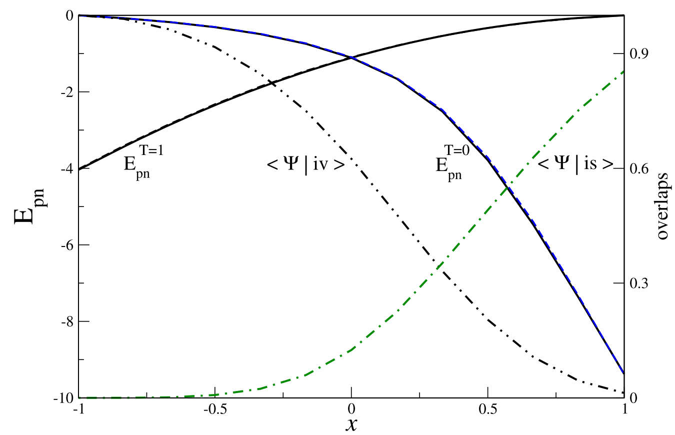

Fig. 1. proton–neutron pairing energies provided by the PQCM approach (full lines) and by exact diagonalization (dashed lines) together with the overlaps between the ground state (5) and the states (7) and (8). The parameter x on horizontal axis scales the strength of the interactions in the two pairing channels (see the text). The results correspond to 4 proton–neutron pairs moving in 10 equidistant levels and the pairing energies are given in units of levels spacing.

the isovector quartet with the two isoscalar pairs. Moreover, one should also consider the fact that the two states (7) and (8) are not orthogonal to each other (see below). Because of these reasons the proton–neutron pairing energies $E_{pn}^{T=0,1}$ have contributions from both the isovector and the isoscalar degrees of freedom. Therefore the pairing energies and the so-called “number of pairs”, which are proportional to the former in the case of state-independent pairing forces, cannot be used as relevant quantities for disentangling the isovector and the isoscalar pairing correlations.

Next we apply the present formalism to analyze the competition between $T = 1$ and $T = 0$ pairing in realistic calculations. As an example we consider $N = Z$ nuclei with the valence nucleons moving outside the closed cores ^{16}O, ^{40}Ca and ^{100}Sn. The single-particle states are generated by Skyrme–HF calculations performed for axially deformed mean fields. In the Skyrme–HF calculations, done with the code *ev*8 [18], we use the force *Sly*4 [19] and we disregard the Coulomb interaction. As the model space for the valence nucleons we consider 10 single-particle levels above the closed cores mentioned above. Since the mean field is axially symmetric, the levels are double degenerate over the projection of the angular momentum on z-axis. In addition, because we neglect the Coulomb interaction, the levels are also degenerate in isospin.

How to fix the pairing interactions in the two pairing channels is a debated issue. Here we shall use the prescriptions suggested in Refs. [4,20,21]. Thus, for the pairing force we take a zero range delta interaction $V^{T=0,1}(\vec{r}_1,\vec{r}_2) = V_0^{T=0,1}\delta(\vec{r}_1-\vec{r}_2)$. The matrix elements of this interaction in the isovector and isoscalar channels are calculated by projecting out from the two-body wave function the component with the total spin $S = 0$ and, respectively, with $(S = 1, S_z = 0)$. The strength of the force in the two channels is taken as $V_0^{T=1} = V_0$ and $V_0^{T=0} = wV_0$. Since the values of the constants V_0 and w are also a matter of debate, we have done calculations with various parameters, i.e., $V_0 = \{300, 465, 720\}$ and $w = \{1, 1.25, 1.5, 175\}$. Because the conclusions relevant for this study are similar in all these calculations, below we are presenting only the results for $V_0 = 465$ and $w = 1.5$, which are the values suggested, respectively, in Ref. [20] and Ref. [4].

The results of the calculations are displayed in Table 1. In the second and third columns are given the pairing correlation energies obtained from exact diagonalization and from PQCM. The correlation energies are defined as the difference between the total energy and the energy obtained in the absence of the interaction. One can observe that for all nuclei the agreement between the

Table 1
Correlation energies calculated in the PQCM approach compared to the exact results. Are shown also the correlation energies obtained by minimizing the Hamiltonian (1) with the isovector $|iv\rangle$ and isoscalar $|is\rangle$ states defined by Eqs. (7), (8). In the last column are given the overlaps between these states.

	Exact	$\|PQCM\rangle$	$\|iv\rangle$	$\|is\rangle$	$\langle iv\|is\rangle$
^{20}Ne	11.38	11.38 (0.00%)	11.31 (0.62%)	10.92 (4.00%)	0.976
^{24}Mg	19.32	19.31 (0.03%)	19.18 (0.74%)	18.93 (2.00%)	0.980
^{28}Si	18.74	18.74 (0.01%)	18.71 (0.14%)	18.54 (1.07%)	0.992
^{44}Ti	7.095	7.094 (0.02%)	7.08 (0.18%)	6.30 (10.78%)	0.928
^{48}Cr	12.78	12.76 (0.1%)	12.69 (0.67%)	12.22 (4.37%)	0.936
^{52}Fe	16.39	16.34 (0.26%)	16.19 (1.17%)	15.62 (4.65%)	0.946
^{104}Te	4.53	4.52 (0.06%)	4.49 (0.82%)	4.02 (11.26%)	0.955
^{108}Xe	8.08	8.03 (0.61%)	7.96 (1.45%)	6.75 (16.47%)	0.814
^{112}Ba	9.36	9.27 (0.93%)	9.22 (1.43%)	7.50 (19.81%)	0.784

exact and the PQCM results is excellent. Similar good agreements we have obtained for the other pairing forces mentioned above. In the columns 4 and 5 are given the results obtained when the minimization of the Hamiltonian (1) is done either with the quartet condensate (7) or the condensate of isoscalar pairs (8). It is surprising to see that the two calculations give results which are not too far from the ones obtained with the full state (5). The fact that the calculations with the states (7) and (8) give comparable results can be understood from the overlap $\langle iv|is\rangle$ shown in the last column of Table 1. One can thus see that this overlap is rather big for all calculated nuclei. From columns (4) and (5) we can notice that for all nuclei the errors corresponding to the calculations done with the quartet condensate (7) are smaller compared to the ones done with the condensate of isoscalar pairs (8), indicating that the isovector pairing correlations are stronger than the isoscalar ones, especially in pf-shell nuclei and in the nuclei above ^{100}Sn. Nonetheless, in all nuclei the isoscalar pairing correlations are significant and, as pointed out by the large overlaps shown in column (6), they cannot be disentangled easily from the isovector pairing correlations.

Finally we would like to mention that the main conclusion of this study, namely the coexistence of the isovector and isoscalar pairing correlations for any $N = Z$ nuclei, refers to pairing forces acting on time-reversed and axially-deformed states. It is however worth mentioning that a similar conclusion was found recently for spherically-symmetric Hamiltonians with $J = 0$ and $J = 1$ pairing forces in which all the components of the isoscalar $J = 1$ pairing force have been taking into account, not only the one scattering pairs in time-reversed states [15]. We recall that in Ref. [15] the isoscalar $J = 1$ pairing is treated by isoscalar quartets built by two $J = 1$ pairs coupled to the total angular momentum $J = 0$. This formalism cannot be applied for the isoscalar pairing interactions acting on deformed states considered in this study since in this case the pairs have not a well-defined angular momentum.

4. Summary

In this Letter we have proposed a new approach for treating the isovector and the isoscalar pairing interactions in axially-deformed $N = Z$ nuclei. In this approach, which conserves exactly the particle number and the isospin, the ground state is constructed as a superposition of condensates formed by isovector quartets and isoscalar pairs. It is shown that this ansatz for the ground state is able to provide very accurate pairing correlation energies for all $N = Z$ nuclei analyzed in this study. One of the important predictions of this formalism is that the isovector and the isoscalar correlations coexist for any pairing interaction. In addition, the realistic calculations presented in this Letter indicate that the isovector and the isoscalar correlations are strongly mixed together and difficult to disentangle from each other.

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