Quartet condensation and isovector pairing correlations in $N = Z$ nuclei

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We propose a simple quartet condensation model (QCM) which describes with very high accuracy the isovector pairing correlations in self-conjugate nuclei. The quartets have an α-like structure and are formed by collective isovector pairs. The accuracy of the QCM is tested for $N = Z$ nuclei for which exact shell model diagonalizations can be performed. The calculations are done with two isovector pairing forces, one extracted from standard shell model interactions and the other of seniority type, acting, respectively, upon spherical and axially deformed single-particle states. It is shown that for all calculated nuclei the QCM gives very accurate values for the pairing correlations energies, with errors which do not exceed 1%. These results show clearly that the correlations induced by the isovector pairing in self-conjugate nuclei are of quartet type and also indicate that QCM is the proper tool to calculate the isovector proton-neutron correlations in mean field pairing models.

Pairing and quantum condensation are outstanding phenomena in many domains of physics. The best known pairing phenomenon is the superconductivity of electrons in metals, described by Bardeen-Cooper-Schrieffer (BCS) theory [1]. For more than 50 years BCS-type approaches have also been applied to describe superfluid properties of atomic nuclei and neutron stars. However, compared to electronic systems, nuclear systems present special features because they involve two kinds of fermions, neutrons and protons. Therefore in nuclear systems one can have not only Cooper pairs of like fermions, such as neutron-neutron (nn) and proton-proton (pp) pairs, but also two types of proton-neutron (pn) pairs, i.e., isovector (isospin $T = 1$) and isoscalar (isospin $T = 0$) pairs. All these pairs should be equally considered in the nuclear systems with the same number of neutrons and protons, which is a difficult task for nuclear microscopical models.

A common approach to treat pairing in $N = Z$ nuclei, where N and Z are the numbers of neutrons and protons, is the generalized Hartree-Fock-Bogoliubov approximation (HFB) [2]. In this approach all types of Cooper pairs are treated in a unified manner but with a trial wave function which does not conserve exactly the particle number and the isospin of the nucleus. Here we shall investigate another approach based not on Cooper pairs but on four-body clusters composed of two neutrons and two protons coupled to the isospin $T = 0$ and to the angular momentum $J = 0$. This four-body structure is commonly called an α-like quartet. The existence of α-like quartets in nuclei is a long standing issue [3]. Quartet structures are also under current investigations in other physical systems, such as spin-3/2 cold fermionic atoms, two band electronic systems, or bilayered systems with particles and holes [4,5].

Various studies have raised the question if a condensate of α-like quartets could exist in the ground state of $N = Z$ nuclei [6–11]. One of the first microscopic models of quartet condensation in nuclei was proposed by Flowers *et al*. [6] and it was based on a BCS-type function written in terms of quartets. Recently a similar calculation scheme was proposed by including in the BCS function both pairs and quartets [11]. A theory of quartet condensation based on a BCS-type function has the advantage of simplicity but its applicability to real nuclei is hindered by the fact that it does not conserve exactly the particle number, which in the case of quarteting is uncertain in groups of four particles at a time. This limitation was discussed extensively in Ref. [10] for the particular case of a degenerate shell. A quartet condensation approach which conserves the number of particles has been proposed in Ref. [7]. In this approach quartets are constructed for each single-particle level, which makes the calculations cumbersome. A more general calculation scheme, based on a simplified version of the quartet model [12] and which works accurately for systems with two quartets outside a closed core, was proposed in Ref. [8]. Quartet condensation was also analyzed in Ref. [9] by considering phenomenological bosons.

The scope of the present Rapid Communication is to introduce a simple quartet condensation model formulated in terms of collective Cooper pairs which is able to describe with a very good accuracy the isovector pairing correlations in nuclei.

The isovector pairing correlations are described by the Hamiltonian

$$\hat{H} = \sum_i \varepsilon_i \left(N_i^\nu + N_i^\pi \right) - \sum_{i,j,\tau} V_{ij} P_{i,\tau}^+ P_{j,\tau}, \qquad (1)$$

where the first term is the single-particle part and the second is the most general isovector interaction. The isovector interaction is invariant under rotations in isospace and it is expressed in terms of the isovector 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 operators ν_i^+ and π_i^+ create, respectively, a neutron and a proton in the state i while $\bar{i}$ denotes the time conjugate of the state i. When all the matrix elements of the interaction are considered of equal strength, the Hamiltonian (1) has SO(5) symmetry and its exact solutions, both for a degenerate and a nondegenerate single-particle spectrum, have been discussed extensively in the literature (e.g., see Refs. [13–16]).

The ground state of the Hamiltonian (1) is described here in terms of α-like quartets. First, we introduce the noncollective quartet operators A_{ij}^+ obtained by coupling two isovector pairs to the total isospin $T = 0$, i.e.,

$$A_{ij}^+ = [P_i^+ P_j^+]^{T=0} = \frac{1}{\sqrt{3}}(P_{i,1}^+ P_{j,-1}^+ + P_{i,-1}^+ P_{j,1}^+ - P_{i,0}^+ P_{j,0}^+). \tag{2}$$

With these operators we construct a collective quartet operator

$$A^+ = \sum_{i,j} x_{ij} A_{ij}^+, \tag{3}$$

where the summation is over the single-particle states included in the calculations.

Finally, with the collective quartet operator we construct the quartet condensate

$$|\Psi\rangle = (A^+)^{n_q}|0\rangle, \tag{4}$$

where n_q is the number of quartets. By construction, this wave function has $N = Z = 2n_q$ and a well-defined total isospin $T = 0$. In addition, if the Hamiltonian (1) has spherical (axial) symmetry, the quartet condensate (4) has also $J = 0$ ($J_z = 0$), where J and J_z are the total angular momentum and its projection on the symmetry axis.

We would like to stress that in this study the word *condensate* means that the function (4) is obtained by applying the same quartet operator many times. Since the quartet operator is a composite fermionic operator, the condensate wave function (4) is not a bosonic condensate of α particles. In fact, the quartets considered in the present model are four-body structures correlated in angular momentum and isospin space rather than tight α clusters correlated in coordinate space.

The calculations with the function (4) can be greatly simplified if we assume that the mixing amplitudes x_{ij} which define the collective quartet operator (3) have a separable form, i.e., $x_{i,j} = x_i x_j$. In this case the collective quartet operator can be written as

$$A^+ = 2\Gamma_1^+ \Gamma_{-1}^+ - (\Gamma_0^+)^2, \tag{5}$$

where $\Gamma_\tau^+ = \sum_i x_i P_{i\tau}^+$ are the collective Cooper pair operators corresponding to the nn, pp, and np pairs. Due to the isospin invariance, all the collective pairs have the same mixing amplitudes x_i. With the operator (5) the state (4) can be written in the following form:

$$\begin{aligned}|\Psi\rangle &= \left(2\Gamma_1^+ \Gamma_{-1}^+ - \Gamma_0^{+2}\right)^{n_q}|0\rangle \\ &= \sum_k \binom{n_q}{k}(-1)^{n_q-k} 2^k (\Gamma_1^+ \Gamma_{-1}^+)^k \Gamma_0^{+2(n_q-k)}|0\rangle. \end{aligned} \tag{6}$$

One can notice that in the expansion above there are two terms which correspond to two particle-number-projected BCS (PBCS) wave functions

$$|\text{PBCS0}\rangle = \Gamma_0^{+2n_q}|0\rangle, \tag{7}$$

$$|\text{PBCS1}\rangle = (\Gamma_1^+ \Gamma_{-1}^+)^{n_q}|0\rangle. \tag{8}$$

The function (7) is a condensate of proton-neutron pairs while the function (8) is a product of a condensate of neutron-neutron pairs with a condensate of proton-proton pairs. Both PBCS functions conserve the number of particles and the projection of the total isospin on the z axis, but they do not have a well-defined total isospin. As seen from the structure of the quartet condensate (6), in order to restore the isospin symmetry one needs to take a combination of all PBCS functions with the number of pairs compatible with the binomial expansion.

The quartet condensate (6) is defined by the mixing amplitudes x_i. They are found from the minimization of the average of the Hamiltonian, $\langle\Psi|H|\Psi\rangle$, and from the normalization condition $\langle\Psi|\Psi\rangle = 1$. The average of the Hamiltonian and the norm are calculated using recurrence relations. This method is based on the relations satisfied by the matrix elements of the pairing interaction between states with an arbitrary number of nn, pp, and np collective pairs defined by

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

As an example, we give below the recurrence relations satisfied by the matrix elements of the operator $P_{i1}^+ P_{j1}$:

$$\begin{aligned}
&\langle n_1 n_2 n_3 | P_{i,1}^+ P_{j,1} | m_1 m_2 m_3 \rangle \\
&= x_i^2 x_j^2 \Big\{ n_1 m_1 n_1 1 m_1 1 \langle n_1 2 n_2 n_3 | P_{j,1}^+ P_{i,1} | m_1 2 m_2 m_3 \rangle + \tfrac{1}{4} n_3 m_3 n_3 1 m_3 1 \langle n_1 n_2 n_3 2 | P_{j,-1}^+ P_{i,-1} | m_1 m_2 m_3 2 \rangle + n_1 m_1 m_3 \\
&\quad \times (n_3 \langle n_1 1 n_2 n_3 1 | P_{j,0}^+ P_{i,0} | m_1 1 m_2 m_3 1 \rangle + n_1 1 \langle n_1 2 n_2 n_3 | P_{j,0}^+ P_{i,1} | m_1 1 m_2 m_3 1 \rangle) + \tfrac{1}{2} n_3 m_1 n_3 1 (m_3 \langle n_1 n_2 n_3 2 | P_{j,0}^+ P_{i,-1} \\
&\quad \times | m_1 1 m_2 m_3 1 \rangle + m_1 1 \langle n_1 n_2 n_3 2 | P_{j,1}^+ P_{i,-1} | m_1 2 m_2 m_3 \rangle) + \delta_{ij} [n_1 n_3 m_1 m_3 (\langle n_1 1 n_2 n_3 1 | m_1 1 m_2 m_3 1 \rangle - \tfrac{1}{2} \langle n_1 1 n_2 n_3 1 | N_i^\nu \\
&\quad + N_i^\pi | m_1 1 m_2 m_3 1 \rangle) + n_1 m_1 n_1 1 m_1 1 (\langle n_1 2 n_2 n_3 | m_1 2 m_2 m_3 \rangle - \langle n_1 2 n_2 n_3 | N_i^\nu | m_1 2 m_2 m_3 \rangle) + \tfrac{1}{4} n_2 m_3 n_3 1 m_3 1 (\langle n_1 n_2 n_3 2 \\
&\quad \times | m_1 m_2 m_3 2 \rangle - \langle n_1 n_2 n_3 2 | N_i^\pi | m_1 m_2 m_3 2 \rangle) - n_1 m_1 (m_3 n_1 1 \langle n_1 2 n_2 n_3 | T_{i,-1} | m_1 1 m_2 m_3 1 \rangle \\
&\quad - n_3 m_1 1 \langle m_1 2 m_2 m_3 | T_{i,-1} | n_1 1 n_2 n_3 1 \rangle) + \tfrac{1}{2} n_3 m_3 (n_3 1 m_1 \langle n_1 n_2 n_3 2 | T_{i,1} | m_1 1 m_2 m_3 1 \rangle + n_1 m_3 1 \langle m_1 m_2 m_3 2 | T_{i,1} | n_1 1 n_2 n_3 1 \rangle)] \Big\} \\
&\quad + m_1 x_j \langle m_1 1 m_2 m_3 | P_{i,1} | n_1 n_2 n_3 \rangle - x_i x_j^2 [n_1 m_1 m_3 \langle m_1 1 m_2 m_3 1 | P_{j,0} | n_1 n_2 n_3 \rangle + n_1 m_1 m_1 1 \langle m_1 2 m_2 m_3 | P_{j,1} | n_1 n_2 n_3 \rangle \\
&\quad + \tfrac{1}{2} n_1 m_3 m_3 1 \langle m_1 m_2 m_3 2 | P_{j,-1} | n_1 1 n_2 n_3 \rangle].
\end{aligned}$$

In the expressions above $T_{i,\tau}$ are the isospin operators and $n_i k$ denotes $n_i - k$ (e.g., $n_i 1 = n_i - 1$). From this example it can be seen that by the recurrence relations are generated not only the matrix elements for the pairing interaction but also for the operators $P_{i,1}^+ P_{j,-1}$, $P_{i,0}^+ P_{j,1}$, $P_{i,0}^+ P_{j,-1}$. The matrix elements of all these operators depend on each other through the recurrence relations satisfied by each of them. More details about the calculation scheme will be given in a forthcoming publication.

It is worth mentioning that the state (4) with the quartet (5) has a similar form with the eigenstate of zero seniority employed in the generalized-seniority model (GSM) of definite isospin [17]. However, since the calculation scheme used here is valid for any isovector pairing interaction while GSM is valid only for the interactions which satisfy specific commutation relations with the pair operators, the present quartet model and the GSM are different, with the former being more general.

The quartet condensation model (QCM) introduced above is applied here with isovector interactions and single-particle spectra commonly used in shell model and mean field calculations (for a preliminary study with schematic spectra, see Ref. [18]). To check the accuracy of QCM we have chosen three sets of $N = Z$ nuclei for which exact shell model calculations can be performed. The three sets of nuclei, shown in Table I between horizontal lines, have the valence nucleons moving outside the double-magic cores ^{16}O, ^{40}Ca, and ^{100}Sn. These cores are considered as inert in the present calculations and the valence nucleons are described with the Hamiltonian (1). First we have applied the QCM for an isovector pairing force extracted from the ($T = 1$, $J = 0$) part of standard shell model interactions acting on spherical single-particle states. More precisely, for the three sets of nuclei shown in Table I we have used, respectively, the following sources for the isovector pairing matrix elements (all other matrix elements were set to zero): (1) a universal sd-shell interaction (USDB) [19] and the energies (in MeV): $\varepsilon_{1d_{5/2}} = -3.926$, $\varepsilon_{2s_{1/2}} = -3.208$, $\varepsilon_{1d_{3/2}} = 2.112$; (2) a monopole-modified Kuo-Brown interaction (KB3G) [20] and the energies $\varepsilon_{1f7/2} = 0.0$, $\varepsilon_{2p3/2} = 2.0$, $\varepsilon_{2p1/2} = 4.0$, $\varepsilon_{1f5/2} = 6.5$; and (3) the effective G-matrix interaction of Ref. [21] and the energies $\varepsilon_{2d_{5/2}} = 0.0$, $\varepsilon_{1g_{7/2}} = 0.2$, $\varepsilon_{2d_{3/2}} = 1.5$, $\varepsilon_{3s_{1/2}} = 2.8$. In order to be able to perform

exact shell model calculations in the major shells $N = 28$–50 and $N = 50$–82, the single-particle states $1g_{9/2}$ and $1h_{11/2}$ were not introduced in the calculations. These limitations do not apply to the quartet model calculations, which can be done for larger $N = Z$ systems than can be presently calculated by the shell model.

The results for the correlations energies, defined as $E_{\mathrm{corr}} = E_0 - E$, where E is the energy of the ground state and E_0 is the energy calculated without taking into account the isovector pairing interaction, are shown in Table I. In the second column the exact shell model results are shown, in the next column the results of QCM, while in the last two column the results of the two PBCS approximations defined by Eqs. (7) and (8) are given. The errors relative to the exact shell model results are given in the parentheses. Concerning the PBCS approximations, it can be seen that the lowest energy is obtained for the state PBCS1 and not for the proton-neutron condensate PBCS0. The latter gives the lowest energy for $N = Z =$ odd systems [22]. It can be also noticed that the errors corresponding to the PBCS approximations are rather large, much larger than for pairing between like particles [23].

The most remarkable result seen in Table I is that QCM gives very small errors, of below 1%, for all the calculated isotopes, including the ones with three and four quartets. It should be mentioned also that QCM calculations are also very fast (a few CPU minutes on an ordinary laptop) and can be applied for nuclei with many proton-neutron pairs, which cannot be calculated with the present SM codes.

An interesting issue is the relation between the QCM and the BCS calculations, called below PBCS(N, T), in which both the particle number and the total isospin are restored using projection techniques. To address this issue we consider here the PBCS(N, T) result for ^{52}Fe shown in Table 3 of Ref. [24]. The PBCS(N, T) calculations are done with an isovector pairing force of constant strength, with a value equal to $g = -24/A$, where A is the mass of the nucleus, and with spherical single-particle states (for details, see Ref. [24]) The correlation energy obtained with the PBCS(N, T) approximation is 7.63 MeV, which should be compared to the exact value, equal to 8.29 MeV. With the same input the correlation energy obtained with the QCM is equal

TABLE I. Correlation energies calculated with isovector pairing forces extracted from standard shell model interactions and with spherical single-particle states. The results correspond to exact shell model diagonalizations (SM), quartet condensation model (QCM), and the two PBCS approximations of Eqs. (7) and (8). Numbers in the parentheses are the errors relative to the exact shell model results.

	SM	QCM	PBCS1	PBCS0
^{20}Ne	9.173	9.170 (0.033%)	8.385 (8.590%)	7.413 (19.187%)
^{24}Mg	14.460	14.436 (0.166%)	13.250 (8.368%)	11.801 (18.389%)
^{28}Si	15.787	15.728 (0.374%)	14.531 (7.956%)	13.102 (17.008%)
^{32}S	15.844	15.795 (0.309%)	14.908 (5.908%)	13.881 (12.389%)
^{44}Ti	5.973	5.964 (0.151%)	5.487 (8.134%)	4.912 (17.763%)
^{48}Cr	9.593	9.569 (0.250%)	8.799 (8.277%)	7.885 (17.805%)
^{52}Fe	10.768	10.710 (0.539%)	9.815 (8.850%)	8.585 (20.273%)
^{104}Te	3.831	3.829 (0.052%)	3.607 (5.847%)	3.356 (12.399%)
^{108}Xe	6.752	6.696 (0.829%)	6.311 (6.531%)	5.877 (12.959%)
^{112}Ba	8.680	8.593 (1.002%)	8.101 (6.670%)	13.064 (13.064%)

TABLE II. Correlation energies calculated with an isovector pairing force of seniority type and with axially deformed single-particle states. The notations are the same as in Table I.

	SM	QCM	PBCS1	PBCS0
^{20}Ne	6.55	6.539 (0.168%)	5.752 (12.183%)	4.781 (27.008%)
^{24}Mg	8.423	8.388 (0.415%)	7.668 (8.963%)	6.829 (18.924%)
^{28}Si	9.661	9.634 (0.279%)	9.051 (6.314%)	8.384 (13.218%)
^{32}S	10.263	10.251 (0.117%)	9.854 (3.985%)	9.372 (18.682%)
^{44}Ti	3.147	3.142 (0.159%)	2.750 (12.615%)	2.259 (28.217%)
^{48}Cr	4.248	4.227 (0.494%)	3.854 (9.275%)	3.423 (19.421%)
^{52}Fe	5.453	5.426 (0.495%)	5.033 (7.702%)	4.582 (15.973%)
^{104}Te	1.084	1.082 (0.184%)	0.964 (11.070%)	0.832 (23.247%)
^{108}Xe	1.870	1.863 (0.374%)	1.697 (9.264%)	1.514 (19.037%)
^{112}Ba	2.704	2.688 (0.592%)	2.532 (6.361%)	2.184 (19.230%)

to 8.25 MeV. This comparison shows that the QCM is much more accurate than PBCS(N, T) and indicates also that QCM describes additional, quartet-type correlations which cannot be obtained in the standard BCS-type models.

In $N = Z$ nuclei there are other important degrees of freedom which compete with the isovector interaction. This can be easily seen from the small overlap between the exact shell model wave functions calculated with the isovector pairing force and with the full two-body interaction. For example, in the case of ^{48}Cr this overlap is equal to 0.614, which is a very small value when compared to similar overlaps calculated for spherical nuclei with like-particle pairing [25]. Among the most important degrees of freedom which compete with the pairing in $N = Z$ nuclei are the quadrupole ones. It has been shown that a simplified model Hamiltonian which includes only the isovector pairing interaction and a quadrupole-quadrupole force is able to give a realistic description of the essential features of $N = Z$ nuclei [26,27]. In the mean field version of this model the quadrupole degrees of freedom are commonly included in a deformed mean field and the isovector pairing is treated in the single-particle basis corresponding to it (e.g., see Ref. [28]). In what follows we use this framework to analyze the quartet correlations in deformed $N = Z$ nuclei. As an illustration we consider the same nuclei shown in Table I. The QCM is applied for an isovector pairing interaction acting on the single-particle spectrum corresponding to an axially deformed mean field. The mean field is generated self-consistently by Hartree-Fock calculations performed with the Skyrme force SLy4 [30] and using the code ev8 [29]. For the isovector pairing force we take a seniority type interaction with the strength $g = -24/A$ [24]. To keep the analogy with the calculations done above for a Hamiltonian with spherical symmetry, the Coulomb interaction is neglected in the mean field and the pairing is applied for the Hartree-Fock (HF) single-particle states above the cores ^{16}O, ^{40}Ca, and ^{100}Sn. More precisely, to be able

to perform exact shell model diagonalizations, for the three sets of nuclei shown in Table I we consider, respectively, the lowest seven, nine, and ten deformed HF single-particle states above the double-magic cores. The results, given in Table II, show that QCM gives very accurate results for a deformed mean field. Although it is not shown, when we vary the interaction strength, from the weak to the strong coupling regime, we continue to get similar very good accuracy. The QCM calculations done in the deformed HF basis conserve the particle number and the total isospin but break the rotation symmetry. Since QCM provides simple rules for evaluating overlaps, the restoration of the rotation symmetry can be done applying standard projection techniques.

In conclusion, we have shown that the isovector pairing correlations in $N = Z$ nuclei are described with a very high accuracy by a condensate of α-like quartets formed by collective pairs. Because of its accuracy and simplicity, the QCM appears to be the appropriate tool for describing the isovector pairing correlations in nuclei.

Finally we would like to mention that due to the general structure of the state (9) employed in the recurrence relations, which is defined for an arbitrary number of pairs, the QCM can be also extended to treat nuclei with a different number of protons and neutrons in the same open shell. The study of quartet correlations in such nuclei is the scope of a future investigation.

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