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Four-nucleon α-type correlations and proton-neutron pairing away from the $N = Z$ line

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We study the competition between α-type and conventional pair condensation in the ground state of nuclei with neutrons and protons interacting via a charge-independent pairing interaction. The ground state is described by a product of two condensates, one of α-like quartets and the other one of pairs in excess relative to the isotope with $N = Z$. It is shown that this ansatz for the ground state gives very accurate pairing correlation energies for nuclei with the valence nucleons above the closed cores ^{16}O, ^{40}Ca, and ^{100}Sn. These results indicate that α-type correlations are important not only for the self-conjugate nuclei but also for nuclei away from the $N = Z$ line. In the latter case α-like quartets coexist with the collective Cooper pairs formed by the nucleons in excess.

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It was suggested long ago that in self-conjugate nuclei proton-neutron pairing can induce, through isospin conservation, four-particle correlations of α type [1]. A related question, repeatedly discussed by various authors, is whether the ground state of $N = Z$ nuclei can be described as a superfluid condensate of α-like quartets. One of the first models of α-type superfluidity in $N = Z$ nuclei was proposed by Flowers *et al.* [2] and it was based on a BCS-like state made of quartets instead of pairs. Recently, this model has been extended by including in the BCS state both quartets and pairs [3]. As any quasiparticle approximation, these models do not conserve exactly the particle number. For α-type correlations this is a serious drawback since in this case the particle number becomes uncertain in units of four particles at a time. α-type condensation in the ground state of $N = Z$ nuclei was also studied in particle-number-conserving models [4–8]. However, the majority of these studies have been done either with schematic single-particle spectra and schematic interactions or using approximations justified for a limited number of quartets. A general calculation scheme for taking into account α-type quartet correlations, valid for any number of quartets and for a general charge-independent pairing force, was proposed recently in Ref. [9]. The calculations done in Ref. [9] show that the isovector pairing correlations in the ground state of $N = Z$ nuclei can be described with high precision by a condensate of α-like quartets built by collective proton-neutron, neutron-neutron, and proton-proton pairs. In this Rapid Communication we shall extend the calculation scheme of Ref. [9] to nuclei away from the $N = Z$ line and we will study to what extent α-like correlations coexist with the conventional pairing in nuclei with excess neutrons or protons. The possibility of coexistence/competition of four-particle correlations of α type with the usual two-body pairing correlations was several times discussed in the literature [3,4,7] but, as far as we know, it was never checked in realistic microscopic calculations.

In the present study we consider a system of N neutrons and Z protons moving outside a self-conjugate core and interacting via a charge-independent pairing force. The corresponding Hamiltonian is

$$\hat{H} = \sum_{i,\tau=\pm 1/2} \varepsilon_{i\tau} N_{i\tau} + \sum_{i,j,t=-1,0,1} V_{ij} P^+_{i,t} P_{j,t}, \tag{1}$$

where $\varepsilon_{i\tau}$ are the single-particle energies associated with the mean fields of neutrons and protons, supposed invariant to time reversal. The isovector interaction 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.

In Ref. [9] the ground state of the Hamiltonian (1) for a system with $N = Z =$ even was described by the trial state

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

where $n_q = (N + Z)/4$ and A^+ is a collective four-nucleon operator defined by

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

A^+_{ij} denotes the noncollective four-nucleon operators constructed by coupling two noncollective isovector pairs to the total isospin $T = 0$; i.e.,

$$A^+_{ij} = [P^+_i P^+_j]^{T=0} = \frac{1}{\sqrt{3}}(P^+_{i,1} P^+_{j,-1} + P^+_{i,-1} P^+_{j,1} - P^+_{i,0} P^+_{j,0}). \tag{4}$$

Supposing that the amplitudes x_{ij} are separable, i.e., $x_{ij} = x_i x_j$, the collective four-nucleon operator (3) can be written as

$$A^+ = 2\Gamma^+_1 \Gamma^+_{-1} - (\Gamma^+_0)^2, \tag{5}$$

where $\Gamma^+_t = \sum_i x_i P^+_{i,t}$ denote, for $t = 0, 1, -1$, the collective pair operators for the proton-neutron (pn), neutron-neutron (nn), and proton-proton (pp) pairs. Due to the isospin invariance, all the collective pairs have the same mixing amplitudes x_i.

With the collective four-nucleon operator (5) the state (2) can be written as

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

From the equation above it can be seen that the α-like condensate for a system with $N = Z =$ even is a particular superposition of nn, pp, and pn pair condensates.

Now we shall consider the case of even-even systems with an excess of one sort of nucleons, neutrons, or protons. For these systems we suppose that the excess neutrons or protons form a pair condensate of conventional type which is appended to the α condensate. Thus, for an even-even system with an excess of neutrons we consider the following ansatz for the ground state:

$$|\Psi\rangle = (\tilde{\Gamma}_1^+)^{n_N}(A^+)^{n_q}|0\rangle = (\tilde{\Gamma}_1^+)^{n_N}\left(2\Gamma_1^+\Gamma_{-1}^+ - \Gamma_0^{+2}\right)^{n_q}|0\rangle, \quad (7)$$

where $n_N = (N-Z)/2$ is the number of neutron pairs in excess and $n_q = (N - 2n_N + Z)/4$ is the maximum number of α-like quartets which can be formed by the neutrons and protons. Since the quartets A^+ have zero isospin, the state (7) has a well-defined total isospin given by the excess neutrons; i.e., $T = n_N$. The neutron pairs in excess are described by the collective pair operator $\tilde{\Gamma}_1^+ = \sum_i y_i P_{i1}^+$. It can be seen that the collective pair describing the excess neutrons is taken of different structure from the collective neutron pair entering in the collective quartet. This is a requirement imposed by the Pauli principle in the HF limit. For the particular case of degenerate single-particle states and a seniority-type pairing force the state (7) is the exact solution of the Hamiltonian (1) [7].

It is important to observe that in the state (7) one can identify two terms which play the role of particle-number-projected BCS (PBCS) approximations for $N > Z$ systems interacting with charge-independent pairing forces; i.e.,

$$|\text{PBCS0}\rangle = (\tilde{\Gamma}_1^+)^{n_N}(\Gamma_0^+)^{2n_q}|0\rangle, \quad (8)$$

$$|\text{PBCS1}\rangle = (\tilde{\Gamma}_1^+)^{N/2}(\Gamma_{-1}^+)^{Z/2}|0\rangle. \quad (9)$$

The state (8) is a product between a condensate of proton-neutron pairs and a condensate of neutron-neutron pairs while the state (9) is a product of a condensate of neutron-neutron pairs with a condensate of proton-proton pairs. Both states have the right number of protons and neutrons but have not a well-defined total isospin.

The mixing amplitudes x_i and y_i which define the ground state (7) are determined from the minimization of $\langle\Psi|H|\Psi\rangle$ under the normalization condition $\langle\Psi|\Psi\rangle = 1$. To calculate the average of the Hamiltonian and the norm we have extended the recurrence relations method of Ref. [9] by including the contribution of the excess neutrons. Thus the recurrence relations are calculated with the following states of arbitrary numbers of collective nn, pp, and np pairs:

$$|n_1n_2n_3n_4\rangle = \Gamma_1^{+n_1}\Gamma_{-1}^{+n_2}\Gamma_0^{+n_3}\tilde{\Gamma}_1^{+n_4}|0\rangle. \quad (10)$$

Compared to $N = Z$ systems, these states have two kinds of neutron collective pairs, corresponding to the extra pairs and to the pairs which are included in the quartet condensate. The recurrence relations satisfied by the matrix elements of the Hamiltonian (1) with the states (10) can be simply related to the recurrence relations we have used in Ref. [9] for $N = Z$ systems. Finally, we would like to stress that in the formalism presented here the Pauli principle is incorporated rigorously, which is very important when four-body correlations are calculated.

The model described above, which will be referred to as quartet condensation model (QCM), as in Ref. [9], is well suited for studying the competition between the α-like four-nucleon correlations and the conventional pairing condensation in nuclei with proton-neutron pairing. As an illustration we apply it here for three sets of nuclei with the valence nucleons moving outside the double-magic cores ^{16}O, ^{40}Ca, and ^{100}Sn, which are taken as inert. For each set of nuclei we start with the $N = Z =$ even isotopes and add extra neutron pairs. The calculations are done for those nuclei for which the ground-state energy can be calculated exactly by diagonalization. To check the accuracy of QCM we have done calculations using for the single-particle energies and the pairing force the two different inputs employed in Ref. [9]. Thus we first applied QCM for a charge-independent pairing interaction of seniority type, with the strength $g = 24/A$, acting on protons and neutrons moving in deformed mean fields. The mean fields are obtained from axially deformed Hartree-Fock (HF) calculations [10] done with the Skyrme force SLy4 [11]. From the HF spectrum of the three sets of

TABLE I. Pairing correlations energies for isotopes having as core ^{16}O. The results correspond to exact diagonalization (Exact), quartet condensation model (QCM), and the PBCS1 approximation (9). Numbers in parentheses are the errors relative to the exact diagonalization. The calculations are done with an isovector pairing force of seniority type and with axially deformed single-particle states.

	Exact	QCM	PBCS1		Exact	QCM	PBCS1
^{20}Ne	6.550	6.539 (0.17%)	5.752 (12.18%)	^{24}Mg	8.423	8.388 (0.41%)	7.668 (8.96%)
^{22}Ne	6.997	6.969 (0.40%)	6.600 (5.67%)	^{26}Mg	8.680	8.654 (0.30%)	8.258 (4.86%)
^{24}Ne	7.467	7.426 (0.55%)	7.226 (3.23%)	^{28}Mg	8.772	8.746 (0.30%)	8.531 (2.75%)
^{26}Ne	7.626	7.592 (0.45%)	7.486 (1.84%)	^{30}Mg	8.672	8.656 (0.18%)	8.551 (1.39%)
^{28}Ne	7.692	7.675 (0.22%)	7.622 (0.91%)	^{32}Mg	8.614	8.609 (0.06%)	8.567 (0.55%)
^{30}Ne	7.997	7.994 (0.04%)	7.973 (0.30%)	^{28}Si	9.661	9.634 (0.28%)	9.051 (6.31%)
^{30}Si	9.310	9.296 (0.15%)	9.064 (2.64%)	^{32}Si	9.292	9.283 (0.10%)	9.196 (1.03%)

TABLE II. The same as in Table I but for isotopes having as core ^{40}Ca and ^{100}Sn.

	Exact	QCM	PBCS1		Exact	QCM	PBCS1
^{44}Ti	3.147	3.142 (0.16%)	2.750 (12.61%)	^{48}Cr	4.248	4.227 (0.49%)	3.854 (9.27%)
^{46}Ti	3.526	3.509 (0.48%)	3.308 (6.18%)	^{50}Cr	4.461	4.444 (0.38%)	4.230 (5.18%)
^{48}Ti	3.882	3.853 (0.75%)	3.735 (3.79%)	^{52}Cr	4.743	4.721 (0.46%)	4.582 (3.39%)
^{50}Ti	3.973	3.956 (0.43%)	3.889 (2.11%)	^{54}Cr	4.869	4.855 (0.29%)	4.772 (1.99%)
^{104}Te	1.084	1.082 (0.18%)	0.964 (11.07%)	^{108}Xe	1.870	1.863 (0.37%)	1.697 (9.25%)
^{106}Te	1.324	1.321 (0.23%)	1.250 (5.59%)	^{110}Xe	2.191	2.185 (0.27%)	2.058 (6.07%)
^{108}Te	1.713	1.698 (0.88%)	1.642 (4.14%)	^{112}Xe	2.449	2.437 (0.49%)	2.348 (4.12%)
^{110}Te	1.892	1.880 (0.63%)	1.843 (2.59%)	^{114}Xe	2.964	2.954 (0.34%)	2.887 (2.60%)

nuclei we consider in the pairing calculations, respectively, the lowest 7, 9, and 10 states above the double-magic core. In the calculations we have neglected the Coulomb interaction and we have used for $N > Z$ nuclei the same single-particle energies as for the corresponding $N = Z$ isotope. As shown in Refs. [12,13], the isospin dependence of the single-particle energies can be eventually taken into account reasonably well by adding to the calculated binding energies a term proportional to $T(T+1)$.

It is important to mention that the Hamiltonian (1) with a similar input as employed here, using deformed mean fields provided by the Nilsson model instead of Skyrme-HF, is realistic enough for describing the experimental even-even to odd-odd energy difference as well as the term linear in *N-Z* (Wigner energy) in the nuclear binding energy [13].

The results we have obtained for pairing correlations energies with the input presented above are shown in Tables I and II. The correlation energies are defined as $E_{\rm corr} = E_0 - E$, where E is the total energy while E_0 is the energy obtained without the pairing interaction. In Tables I and II the QCM results are compared to the exact results, obtained by direct diagonalization, and with the results provided by the PBCS1 approximation (9). Since, as in $N = Z$ systems [9,14], the PBCS0 approximation (8) gives less binding compared to PBCS1, its prediction are not given here.

Two points emerge immediately from Tables I and II. First, it can be noticed that QCM describes with very good accuracy the pairing correlations energies for all calculated isotopes. Thus for all the isotopes the errors relative to the exact results (shown in the parentheses) are below 1%. Second, it can be seen that the PBCS1 approximation, in which it is supposed that the system splits into two superfluids composed by neutrons and protons, is less accurate, much less than the PBCS approximation for like-particle pairing [15]. As expected, its accuracy increases with the number of pairs in excess. Since by adding more and more neutron pairs the role of proton-neutron pairs is diminishing, one may think that there is a phase transition from a mixed condensate of α-like quartets and neutron pairs to a standard mixed condensate of neutrons and protons, as described by the state PBCS1. From the calculations presented in Tables I and II it appears that this is not the case.

Apart from correlation energies, we have also checked that QCM predicts accurate results for occupation probabilities of single-particle states. As an example in Table III are shown the results for the isotope ^{30}Mg.

More specific information about the correlations described by QCM can be extracted from the entanglement properties of the Cooper pairs which compose the ground states (7). As a measure of the entanglement we use here the so-called Schmidt number [16] defined as $K = (\sum_i w_i^2)^2/\sum_i w_i^4$, where w_i are the mixing amplitudes of the two-body function which describes the entangled particles (for an application of Schmidt number to like-particle pairing in nuclei see [15]). In the case of the Cooper pairs Γ_t^+ and $\tilde{\Gamma}_1^+$ the mixing amplitudes w_i are, respectively, x_i and y_i. As expected, the Schmidt numbers show that the entanglement of the proton pairs is stronger when they are included in the quartets than when they form a pair condensate as in PBCS1. For example, in ^{30}Mg we obtain $K = 1.88$ for the protons in the quartet condensate and $K = 1.79$ for the protons in the pair condensate. As for the neutron pairs in excess, they are usually much more entangled than the ones included in the quartets (e.g., by about 64% in ^{30}Mg).

To check further the accuracy of QCM, we have also done calculations with more general isovector pairing forces, extracted from the $(T = 1,\ J = 0)$ part of standard shell model interactions, acting on spherical single-particle states. As an example, in Table IV we present the correlation pairing energies obtained for the nuclei having as closed core ^{100}Sn. One can observe that QCM gives very good predictions, comparable to the calculations done with the seniority-type force presented in Tables I and II. The calculations have been done with the isovector pairing force extracted from the effective *G*-matrix interaction of Ref. [17] and with the single-particle energies $\varepsilon_{2d_{5/2}} = 0.0$, $\varepsilon_{1g_{7/2}} = 0.2$, $\varepsilon_{2d_{3/2}} = 1.5$, $\varepsilon_{3s_{1/2}} = 2.8$. The intruder state $h_{11/2}$ was not introduced in the calculations because with it the exact diagonalizations

TABLE III. Occupation probabilities of single-particle states in ^{30}Mg. Shown are the exact and the QCM results for neutrons (n) and protons (p).

ε_i	Exact(n)	QCM(n)	Exact(p)	QCM(p)
−16.45	0.995	0.995	0.983	0.983
−13.94	0.993	0.993	0.961	0.963
−10.39	0.987	0.987	0.028	0.026
−8.08	0.971	0.972	0.012	0.017
−6.09	0.921	0.923	0.007	0.007
−3.89	0.087	0.085	0.005	0.005
−2.61	0.045	0.045	0.004	0.004

TABLE IV. Pairing correlations energies for isotopes having as core ^{100}Sn calculated with the isovector pairing force extracted from the effective G-matrix interaction of Ref. [17] and with spherical single-particle states. The notations are the same as in Table I.

	Exact	QCM	PBCS1		Exact	QCM	PBCS1
^{104}Te	3.831	3.829 (0.05%)	3.607 (5.85%)	^{108}Xe	6.752	6.696 (0.83%)	6.311 (6.53%)
^{106}Te	5.156	5.130 (0.50%)	4.937 (4.25%)	^{110}Xe	7.578	7.509 (0.91%)	7.184 (5.20%)
^{108}Te	5.970	5.930 (0.67%)	5.768 (3.38%)	^{112}Xe	8.285	8.208 (0.93%)	7.944 (4.12%)
^{110}Te	6.664	6.616 (0.72%)	6.485 (2.69%)	^{114}Xe	8.446	8.368 (0.92%)	8.167 (3.30%)
^{112}Te	6.815	6.764 (0.75%)	6.665 (2.20%)	^{116}Xe	8.031	7.947 (1.05%)	7.810 (2.75%)

cannot be performed due to the very large matrices (e.g, 186 billion for ^{116}Xe). It is worth mentioning that the intruder state, which has a significant influence for the heavier isotopes shown in Table IV, can be simply accounted for in QCM. In fact, as any approach based on variational principle, the QCM can be applied for nuclei and model spaces which are far beyond the capability of present shell model codes.

To conclude, in this Rapid Communication we have shown that four-nucleon correlations of α type are very important in systems with neutron-proton pairing. This is true not only for systems with $N = Z$ but also for systems with excess neutrons. It means that, whenever possible, the protons and neutrons prefer to couple together in α-like quartets which are forming an α-like condensate. When not all neutrons can be included in the α-like quartets, the excess neutrons form a typical condensate of collective pairs which is appended to the α-like condensate. We have found that the α-type correlations coexist with the conventional pairing of excess neutrons irrespective to the number of excess neutrons. To the best of our knowledge, these are the first realistic microscopic calculations which point to the coexistence of α-like quartets and conventional Cooper pairs in nuclei away from the $N = Z$ line.

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