

Isovector pairing in a formalism of quartets for $N = Z$ nuclei

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We describe the ground state of the isovector pairing Hamiltonian in self-conjugate nuclei by a product of collective quartets of different structures built from two neutrons and two protons coupled to total isospin $T = 0$. The structure of the collective quartets is determined by an iterative variational procedure based on a sequence of diagonalizations of the pairing Hamiltonian in spaces of reduced size. The accuracy of the quartet model is tested for $N = Z$ nuclei carrying valence nucleons outside the ^{16}O , ^{40}Ca , and ^{100}Sn cores. The comparison with the exact solutions of the pairing Hamiltonian, obtained by shell model diagonalization, shows that the quartet model is able to describe the isovector pairing energy with very high precision. The predictions of the quartet model are also compared to those of the simpler quartet condensation model in which all the collective quartets are assumed to be identical.

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In self-conjugate nuclei the isovector proton-neutron pairing is expected to coexist in an equal amount with the neutron-neutron and proton-proton pairings, as a consequence of isospin invariance of nuclear forces [1]. The most common approach employed to treat the isovector pairing in these nuclei is the generalized BCS model [2–4]. In this approach, however, the proton-neutron pairs do not coexist with the like-particle pairs. More precisely, in BCS one usually gets two degenerate solutions for the ground state of nuclei with $N = Z$, namely a solution with only proton-neutron pairs and a solution with only like-particle pairs [4,5]. As can be seen from the comparison with exactly solvable SO(5) pairing models, the two BCS solutions do not mix with each other because of the isospin symmetry breaking [6,7]. On the other hand, restoring the isospin symmetry in BCS-like models is not enough to obtain a proper description of the isovector pairing correlations even if, in addition, particle number conservation is also restored [8]. This fact indicates the need for a more general isospin-conserving formalism which goes beyond the BCS-based approximations. One such formalism, explored in Ref. [8], is the generator coordinate method (GCM) applied on a projected BCS state. An alternative approach, proposed recently in Refs. [9,10], describes the isovector pairing correlations in terms of a condensate of identical α -like quartets built by two neutrons and two protons coupled to a total isospin $T = 0$. The aim of this study is to propose a more general quartet model approach in which the isovector pairing in the ground state of $N = Z$ nuclei is described not as a condensate of identical quartets but as a product of quartets all having different structures. It will be shown that by this extension the quartet model gives results which reproduce almost exactly the solutions of realistic isovector pairing Hamiltonians.

The isovector pairing correlations are described by the Hamiltonian

$$\hat{H} = \sum_i \epsilon_i (N_i^v + N_i^\pi) + \sum_{i,j} V_{ij} \sum_{\tau} P_{i,\tau}^+ P_{j,\tau}. \quad (1)$$

In the first term the operators N_i^v and N_i^π are, respectively, the neutron and proton number operators and ϵ_i are the single-particle energies. Because in this study we treat only systems with $N = Z$ and since the Coulomb force is not taken into account, the single-particle energies are considered to be the same for both protons and neutrons. The pairing interaction is written in terms of the pair operators

$$P_{i,\tau}^+ = [a_i^+ a_{\bar{i}}^+]_{\tau}^{T=1} \quad (2)$$

where \bar{i} stands for the time conjugate of the state i and τ denotes the three projections of the isospin $T = 1$ corresponding to neutron-neutron ($\tau = 1$), proton-proton ($\tau = -1$), and proton-neutron ($\tau = 0$) pairs. The Hamiltonian (1) with a state-independent interaction strength, i.e., $V_{ij} = g$, can be solved analytically [11–14].

To describe the ground state of the Hamiltonian (1) for systems with $N = Z$ we use as building blocks not Cooper pairs, as done in BCS-type models, but collective quartets formed by two neutrons and two protons. Thus, we first introduce a set of noncollective quartets composed by two isovector pairs coupled to $T = 0$:

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

With these noncollective quartets we then construct the collective quartets:

$$Q_v^+ = \sum_{i,j} q_{ij}^{(v)} A_{ij}^+. \quad (4)$$

Finally, with these collective quartets, we define the state

$$|\Psi_{gs}\rangle = \prod_{v=1}^N Q_v^+ |0\rangle. \quad (5)$$

This quartet state provides our ansatz for the ground state of the isovector pairing Hamiltonian (1) in the case of even-even proton-neutron systems with $N = Z$. It is worth mentioning

that the present quartet model is different from the roton model of Arima and Gillet [15] whose quartets, as well as the proton and neutron pairs explicitly forming them, are allowed to couple to any angular momentum. Due to such a feature, the roton model appears to be more suited to describe the quarteting in heavy deformed nuclei where protons and neutrons occupy different valence shells and the proton-neutron pairing is not expected to play any important role.

The quartet state (5) depends on the mixing amplitudes which define the collective quartets (4). In order to search for the most appropriate $q_{ij}^{(v)}$'s we make use of an iterative variational procedure. This procedure is basically identical to that we have recently used in the case of like-particle quartets [16] and draws inspiration from an analogous technique previously developed for a treatment of pairing correlations in terms of a set of independent pairs [17]. The procedure consists of a sequence of diagonalizations of the Hamiltonian in spaces of a rather limited size. In more detail, let us suppose that, at a given stage of the iterative process, one knows the state (5). Let us construct the space

$$F_N^{(\rho)} = \left\{ [P_i^\dagger P_j^\dagger]^{T=0} \prod_{v=1(v \neq \rho)}^{N-1} Q_v^\dagger |0\rangle \right\}_{1 \leq i < j \leq \Omega} \quad (6)$$

(Ω being the number of single-particle states). The states of $F_N^{(\rho)}$ are generated by acting with the operators $[P_i^\dagger P_j^\dagger]^{T=0}$ on the product of all the quartets Q_v^\dagger but the ρ th one. The dimension of each space (6) is therefore at most $\Omega(\Omega + 1)/2$ and one can form N such spaces. By diagonalizing the Hamiltonian in $F_N^{(\rho)}$ and searching for the lowest eigenstate, one constructs the state

$$|\Psi_{gs}^{(new)}\rangle = Q_\rho^{(new)\dagger} \prod_{v=1(v \neq \rho)}^{N-1} Q_v^\dagger |0\rangle. \quad (7)$$

This differs from $|\Psi_{gs}\rangle$ only for the new quartet $Q_\rho^{(new)\dagger}$ and its energy is by construction lower than (or, at worst, equal to) that of $|\Psi_{gs}\rangle$. As a result of this operation, the quartet $Q_\rho^{(new)\dagger}$ has updated Q_ρ^\dagger while all the other quartets have remained unchanged. At the same time the energy of $|\Psi_{gs}\rangle$ has been driven towards its minimum. Performing a series of diagonalizations of H in $F_N^{(\rho)}$ for all possible ρ values ($1 \leq \rho \leq N$) exhausts what we define as an alternative cycle. At the end of a cycle all the quartets Q_v^\dagger have been updated and a new cycle can then start. The sequence of iterative cycles goes on until the difference between the ground-state energy at the end of two successive cycles becomes vanishingly small. In practice, in order to describe a system with N quartets, one proceeds step-by-step starting from the case of just one quartet. The diagonalization of H in the space $F_1^{(1)}$, which simply consists of the states $[P_i^\dagger P_j^\dagger]^{T=0}|0\rangle$, generates Q_1^\dagger . For $N = 2$, the diagonalization in $F_2^{(2)}$, with Q_1^\dagger taken from the previous calculation, generates the first approximation of the quartet Q_2^\dagger . Iterating these diagonalizations in $F_2^{(1)}$ and $F_2^{(2)}$ gives rise to the final quartets Q_1^\dagger and Q_2^\dagger for $N = 2$. Similarly, for $N = 3$, the diagonalization in $F_3^{(3)}$, with Q_1^\dagger and Q_2^\dagger taken from the

previous calculation, generates the first approximation of the quartet Q_3^\dagger , and so on.

In the quartet state (5) the quartets are different from one another. A simpler approach, to which the quartet model will be compared below, simply assumes that all quartets have the same structure [9]. In this approach, called the quartet condensation model, the ground state is therefore approximated by the quartet condensate

$$|\Psi\rangle = (A^+)^N |0\rangle, \quad (8)$$

where A^+ is the collective quartet defined by

$$A^+ = \sum_{i,j} x_{ij} A_{ij}^+ \quad (9)$$

To make possible the connection to the Cooper pairs used in BCS-type models, in Ref. [9] it was supposed that the mixing amplitudes of the collective quartet (9) are separable, i.e., $x_{i,j} = x_i x_j$. With this approximation the collective quartet can be written as

$$A^+ = 2\Gamma_1^+ \Gamma_{-1}^+ - (\Gamma_0^+)^2, \quad (10)$$

where $\Gamma_t^+ = \sum_i x_i P_{i,t}^+$, for $t = 0, 1, -1$, denote the collective pair operators for the proton-neutron, neutron-neutron, and proton-proton pairs, respectively. Due to the isospin invariance, all the collective pairs have the same mixing amplitudes x_i . They are determined by minimizing the average of the Hamiltonian (1) with the normalization constraint. The details of the calculations can be found in Ref. [9].

To test the accuracy of the quartet model we have performed calculations for three sets of $N = Z$ nuclei with valence nucleons outside the cores ^{16}O , ^{40}Ca , and ^{100}Sn . Following Ref. [9], we have performed calculations with two different inputs for the isovector pairing Hamiltonian (1) and chosen only the $N = Z$ systems for which the Hamiltonian can be diagonalized exactly. We have first considered the case of spherically symmetric single-particle states and isovector pairing forces extracted from the ($T = 1, J = 0$) part of standard shell model interactions. Namely, for the three sets of nuclei mentioned above we have extracted the isovector pairing force from the universal sd-shell interaction (USDB) [18], the monopole-modified Kuo-Brown interaction (KB3G) [19], and the effective G -matrix interaction of Ref. [20]. Details about the single-particle energies employed in the calculations are given in Ref. [9]. The results for the pairing correlations energies, defined as the difference between the ground-state energies obtained without and with the pairing force, are given in Table I. The correlation energies predicted by the quartet model (QM) are compared to the exact results and the results of quartet condensation model (QCM). The QCM results and the exact results [21] are extracted from Ref. [9]. We notice that for the systems with one quartet outside the closed core the quartet state (5) is by construction exact. This is not the case for the quartet condensate state (8) because of the factorization approximation $x_{ij} = x_i x_j$. For systems with more than one quartet outside the core, the quartet state (5) is not exact anymore. However, as seen in Table I, the errors relative to the exact solution are very small. We can also observe that the QM gives smaller errors than QCM, reflecting the gain in

TABLE I. Correlation energies for spherical single-particle states and pairing forces extracted from standard shell-model interactions. The results are shown for the exact diagonalizations, the quartet model (QM), and the quartet condensation model (QCM) of Ref. [9]. In parentheses we give the errors relative to the exact results.

	Exact	QM	QCM
²⁰ Ne	9.174	9.174 (—)	9.170 (0.04%)
²⁴ Mg	14.461	14.458 (0.02%)	14.436 (0.17%)
²⁸ Si	15.787	15.780 (0.04%)	15.728 (0.37%)
³² S	15.844	15.844 (—)	15.795 (0.31%)
⁴⁴ Ti	5.965	5.965 (—)	5.964 (0.02%)
⁴⁸ Cr	9.579	9.573 (0.06%)	9.569 (0.10%)
⁵² Fe	10.750	10.725 (0.23%)	10.710 (0.37%)
¹⁰⁴ Te	3.832	3.832 (—)	3.829 (0.08%)
¹⁰⁸ Xe	6.752	6.752 (—)	6.696 (0.83%)
¹¹² Ba	8.680	8.678 (0.02%)	8.593 (1.00%)

correlation energy obtained in QM by allowing the quartets to be different.

We have also tested the accuracy of the quartet model for an isovector pairing interaction acting on the single-particle spectrum corresponding to an axially deformed mean field. As in Ref. [9], the single-particle energies have been extracted from axially deformed Skyrme-HF calculations performed with the force SLy4 [22] and neglecting the Coulomb interaction. For the isovector pairing force we have taken a state-independent interaction with strength $g = 24/A$ (A being the mass number of the nucleus). As in the case of spherical symmetry, the pairing has been applied to the nucleons outside the cores ¹⁶O, ⁴⁰Ca, and ¹⁰⁰Sn. In the calculations, we have considered the lowest seven, nine, and ten HF single-particle states, respectively, above the cores just mentioned. The numbers of these states have been chosen to keep the total degeneracy of the model space approximately the same as in the case of spherical calculations. The results are presented in Table II. In this case the correlation energies predicted by the quartet model are basically exact. The same high precision has been observed for the occupation probabilities.

In order to test its accuracy, the quartet model has been applied here only to $N = Z$ systems for which the Hamiltonian (1) can be diagonalized exactly by shell model techniques. However, we remark that, being based on diagonalizations of matrices of reduced size and also involving a model space much smaller than the full shell model space, the quartet model lends itself to the treatment of $N = Z$ nuclei with more

TABLE II. Correlation energies calculated for axially deformed single-particle states and a state-independent isovector pairing force. The results are shown for the exact diagonalizations, the quartet model (QM), and the quartet condensation model (QCM) of Ref. [9]. In parentheses we give the errors relative to the exact results.

	Exact	QM	QCM
²⁰ Ne	6.5505	6.5505	6.539 (0.18%)
²⁴ Mg	8.4227	8.4227	8.388 (0.41%)
²⁸ Si	9.6610	9.6610	9.634 (0.28%)
³² S	10.2629	10.2629	10.251 (0.12%)
⁴⁴ Ti	3.1466	3.1466	3.142 (0.15%)
⁴⁸ Cr	4.2484	4.2484	4.227 (0.50%)
⁵² Fe	5.4532	5.4531	5.426 (0.50%)
¹⁰⁴ Te	1.0837	1.0837	1.082 (0.16%)
¹⁰⁸ Xe	1.8696	1.8696	1.863 (0.35%)
¹¹² Ba	2.7035	2.7034	2.688 (0.57%)

valence nucleons and/or larger shells than in standard shell model calculations. In addition, the quartet model provides a deeper insight into the structure of the ground-state wave function.

In conclusion, in this study we have proposed a quartet model for the ground state of the isovector pairing Hamiltonian in self-conjugate nuclei. This model assumes that the ground state of even-even systems with $N = Z$ is a product of collective, distinct $T = 0$ quartets built by two neutrons and two protons. The collective quartets are determined by an iterative variational procedure. The calculations carried out for various isovector pairing Hamiltonians have shown that the quartet model reproduces with very high precision the ground-state correlation energies of these systems. This model therefore is an appropriate tool for the treatment of the isovector pairing in mean-field-type models. We also emphasize that the quartet formalism discussed in this work can be extended in a straightforward way to the treatment of more complex Hamiltonians such as, for instance, the isovector plus isoscalar pairing Hamiltonian. Work is in progress in this direction.

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