Isovector pairing in self-conjugate nuclei in a formalism of quartets

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Abstract. The isovector proton-neutron pairing in self-conjugate nuclei is treated in a formalism of quartets. Quartets are four-body correlated structures built from two neutrons and two protons coupled to total isospin $T = 0$. The ground state of the isovector pairing Hamiltonian is described as a product of quartets. We review both the case in which the quartets are constrained to be all identical and the case in which they are allowed to be distinct from one another. The quality of the two approaches is tested by making comparisons with exact shell model calculations for $N = Z$ nuclei with valence nucleons outside the $^{16}$O, $^{40}$Ca, and $^{100}$Sn cores. We consider both spherical and axially deformed mean fields. Both approaches are found to be very accurate. In the applications to a deformed mean field, in particular, the formalism with distinct quartets gives rise to results which are basically exact.

1. Introduction

In self-conjugate nuclei protons ($p$) and neutrons ($n$) occupy the same orbitals. Owing to this fact and to the charge independence of the nuclear force, one expects that in these nuclei the isovector $pn$ pairing should exist on an equal footing with the isovector $pp$ and $nn$ pairing. Extending traditional approaches to pairing like BCS or projected-BCS to $pn$ systems has not led to a satisfactory description of the isovector pairing \cite{1, 2, 3, 4}. An important limitation of these approaches is that they violate isospin symmetry. However, restoring this symmetry has not been sufficient to obtain a proper description of the isovector pairing correlations even in the presence of particle number conservation \cite{5}. This fact indicates the need for a more general isospin conserving formalism which goes beyond the BCS-based approximations.

The isovector pairing ground state in BCS-like approaches is described in terms of collective $pp$, $nn$ and $pn$ pairs. Recently, an alternative approach has been proposed \cite{6} which is instead based on four-body correlated structures formed by two protons and two neutrons coupled to a total isospin $T = 0$ (quartets). In this approach, named quartet condensation model (QCM), the ground state of a self-conjugate nucleus is simply described as a product of identical quartets. The structure of these quartets is determined by minimizing the ground state energy. This approach has been afterwards generalized by allowing the quartets to be all distinct from one another \cite{7}. In this case, in order to construct the quartets, use is done of an iterative procedure based on the diagonalization of the Hamiltonian in restricted spaces. In the following, this approach will be referred to as quartet model (QM). Both QCM and QM have been tested by
making comparisons with exact shell model calculations for \( N = Z \) nuclei with valence nucleons outside the \(^{16}\text{O}, \, ^{40}\text{Ca}, \, ^{100}\text{Sn}\) cores for both spherical and axially deformed mean fields. These comparisons will be illustrated in section 3. Before that, in section 2, we will shortly present the quartet formalism. Finally, in section 4, we will give some conclusions.

2. The quartet formalism

The isovector pairing Hamiltonian has the form

\[
H = \sum_i \epsilon_i (N_i^\nu + N_i^\pi) + \sum_{i,j} V_{ij} \sum_{\tau} P_{i,\tau}^+ P_{j,\tau}^-
\]  

(1)

with the operators \( N_i^\nu \) and \( N_i^\pi \) being, respectively, the neutron and proton number operators, \( \epsilon_i \) the single-particle energies and

\[
P_{i,\tau}^+ = [a_{i} a_{i}]_{T=1}^\tau.
\]

(2)

In the pair creation operator (2), \( \bar{i} \) stands for the time conjugate of the state \( i \) and \( \tau \) denotes the three projections of the isospin \( T = 1 \) corresponding to \( nn \) (\( \tau = 1 \)), \( pp \) (\( \tau = -1 \)) and \( pn \) (\( \tau = 0 \)) pairs.

To describe the ground state of the Hamiltonian (1) for systems with \( N = Z \) we shall use as building blocks not collective pairs, as done in BCS-type models, but collective quartets formed by two neutrons and two protons. To such a purpose, let’s first introduce a set of non-collective quartets composed by two isovector pairs coupled to \( T = 0 \)

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

(3)

The collective quartets are defined as linear combinations of the quartet operators (3)

\[
Q_{\nu}^+ = \sum_{i,j} q_{ij}^{(\nu)} A_{ij}^+.
\]

(4)

By construction, each quartet has a total isospin \( T = 0 \). In addition, if the Hamiltonian (1) has spherical (axial) symmetry, \( Q_{\nu}^+ \) has also \( J = 0 \) (\( J_z = 0 \)), where \( J \) and \( J_z \) are the total angular momentum and its projection on the symmetry axis.

For a self-conjugate nucleus with \( N = Z \equiv 2n \), the QCM assumes that the ground state is formulated in terms of just one collective quartet, say \( Q^+ \), as [6]

\[
|\Psi^{(QCM)}\rangle = (Q^+)^n |0\rangle.
\]

(5)

The mixing amplitudes defining the quartet \( Q^+ \) are determined by minimizing the expectation value of \( H \) in the state \( |\Psi^{(QCM)}\rangle \) properly normalized. Assuming that the coefficients \( q_{ij} \) of \( Q^+ \) have a separable form, i.e. \( q_{ij} \equiv q_i q_j \), allows the use of recurrence relations which greatly facilitate the evaluation of this expectation value [6]. With this approximation the collective quartet can be written as

\[
Q^+ = 2 \Gamma_{+}^+ \Gamma_{-}^+ - (\Gamma_{0}^+)^2,
\]

(6)

where \( \Gamma_{\nu}^+ = \sum_i q_i P_{i,\tau}^+ \). Due to the isospin invariance, all the collective pairs have the same mixing amplitudes \( q_i \).

According to QM, instead, the isovector pairing ground state has the form [7]

\[
|\Psi^{(QM)}\rangle = \prod_{\nu=1}^{n} Q_{\nu}^+ |0\rangle.
\]

(7)
In order to search for the most appropriate \( q_{ij}^{(\nu)} \)'s we make use of an iterative variational procedure which is derived from an analogous treatment of like-particle pairing in terms of independent pairs [8]. The procedure consists of a sequence of diagonalizations of the Hamiltonian in spaces of a rather limited size. Each diagonalization allows to update one quartet while leaving the others unchanged and it drives the ground state toward its minimum. No approximations on the mixing amplitudes \( q_{ij}^{(\nu)} \) are introduced in this case.

3. Results
To test the accuracy of the quartet approaches we have performed calculations for three sets of \( N = Z \) nuclei with valence nucleons outside the cores \(^{16}\text{O}, ^{40}\text{Ca}, \) and \(^{100}\text{Sn} \). 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. Details about the single-particle energies employed in the calculations are given in Refs. [6, 7]. The results for the pairing correlation energies, defined as the difference between the ground state energies obtained without and with the pairing force, are given in Table 1.

Table 1. 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 QM and the QCM. In brackets we give the errors relative to the exact results.

| \( ^{20}\text{Ne} \) | Exact | QM | QCM |
|---|---|---|---|
| 9.174 | 9.174 (-) | 9.170 (0.04%) |
| \( ^{24}\text{Mg} \) | 14.461 | 14.458 (0.02%) | 14.436 (0.17%) |
| \( ^{28}\text{Si} \) | 15.787 | 15.780 (0.04%) | 15.728 (0.37%) |
| \( ^{32}\text{S} \) | 15.844 | 15.844 (-) | 15.795 (0.31%) |

| \( ^{44}\text{Ti} \) | 5.965 | 5.965 (-) | 5.964 (0.02%) |
| \( ^{48}\text{Cr} \) | 9.579 | 9.573 (0.06%) | 9.569 (0.10%) |
| \( ^{52}\text{Fe} \) | 10.750 | 10.725 (0.23%) | 10.710 (0.37%) |

| \( ^{100}\text{Te} \) | 3.832 | 3.832 (-) | 3.829 (0.08%) |
| \( ^{108}\text{Xe} \) | 6.752 | 6.752 (-) | 6.696 (0.83%) |
| \( ^{112}\text{Ba} \) | 8.680 | 8.678 (0.02%) | 8.593 (1.00%) |

In this table the correlation energies predicted by QM and QCM are compared to the exact results. We notice that for the systems with one quartet outside the closed core the state (7) is by construction exact. This is not the case for the quartet condensate (5) because of the factorization approximation \( q_{ij} = q_i q_j \). Both QM and QCM results are characterized by very small errors, with those of QM being always smaller. This reflects the gain in correlation energy obtained in QM by allowing the quartets to be different.

We have also tested the accuracy of the quartet approaches for an isovector pairing interaction acting on the single-particle spectrum corresponding to an axially deformed mean field. The single-particle energies have been extracted from axially deformed Skyrme-HF calculations performed with the force SLy4 and neglecting the Coulomb interaction. For the isovector pairing force we have taken a state-independent interaction with strength \( g = 24/A \). As in the case of spherical symmetry, the pairing has been applied to the nucleons outside the cores \(^{16}\text{O}, ^{40}\text{Ca}, \) and \(^{100}\text{Sn} \). In the calculations we have considered, respectively, the lowest seven, nine, and ten HF single-particle states above the cores just mentioned. The number of these states has been chosen such as 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 2. One still observes a
Table 2. 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 QM and the QCM. In brackets 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%) |

very good performance of QCM and an even improved one by QM whose predictions are, in this case, basically exact. The same high precision is observed for the occupation probabilities.

4. Conclusions
We have provided a description of the ground state of an isovector pairing Hamiltonian in a formalism of quartets. We have discussed two approaches, one describing the ground state as a product of identical quartets and the other allowing the quartets to be all distinct from one another. We have tested these approaches by carrying out a number of comparisons with exact shell model calculations. Both approaches have been found to be very accurate. The one corresponding to distinct quartets, in particular, has provided results basically exact in the applications to an axially deformed mean field. These results strongly support the conclusion that $T = 0$ quartets are appropriate tools for the treatment of the isovector pairing in self-conjugate nuclei.

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