# Isovector and isoscalar pairing in odd-odd N = Z nuclei within a quartet approach

D. Negrea<sup>1,\*</sup>, N. Sandulescu<sup>1,\*</sup>, and D. Gambacurta<sup>2,\*</sup>

<sup>1</sup>National Institute of Physics and Nuclear Engineering, 76900 Bucharest-Magurele, Romania <sup>2</sup>Extreme Light Infrastructure—Nuclear Physics (ELI-NP), 76900 Bucharest-Magurele, Romania \*E-mail: negrea.daniel@theory.nipne.ro; sandulescu@theory.nipne.ro; danilo.gambacurta@eli-np.ro

Received February 21, 2017; Revised April 27, 2017; Accepted April 28, 2017; Published July 29, 2017

The quartet condensation model (QCM) is extended to the treatment of isovector and isoscalar pairing in odd–odd N = Z nuclei. In the extended QCM approach the lowest states of isospin T = 1 and T = 0 in odd–odd nuclei are described variationally by trial functions composed of a proton–neutron pair appended to a condensate of 4-body operators. The latter are taken as a linear superposition of an isovector quartet, built by two isovector pairs coupled to the total isospin T = 0, and two collective isoscalar pairs. In all pairs the nucleons are distributed in time-reversed single-particle states of axial symmetry. The accuracy of the trial functions is tested for realistic pairing Hamiltonians and odd–odd N = Z nuclei with the valence nucleons moving above the <sup>16</sup>O, <sup>40</sup>Ca, and <sup>100</sup>Sn cores. It is shown that the extended QCM approach is able to predict with high accuracy the energies of the lowest T = 0 and T = 1 states. The present calculations indicate that in these states the isovector and isoscalar pairing correlations coexist, with the former playing a dominant role.

.....

Subject Index D10, D11

## 1. Introduction

Recently, many experimental and theoretical studies have been dedicated to the role played by the isoscalar and isovector proton-neutron (pn) pairing in odd-odd N = Z nuclei (see, e.g., Refs. [1,2] and references therein). The experimental data show that the ground states of odd-odd N = Z nuclei have the isospin T = 0 for A < 34 and, with some exceptions, the isospin T = 1 for heavier nuclei. This fact is sometimes considered as an indication of the dominant role of isoscalar (T = 0) pn pairing in light N = Z nuclei. The fingerprints of T = 0 pn pairing in odd-odd N = Z nuclei have also been investigated recently in relation to the Gamow-Teller (GT) charge-exchange reactions. Thus in some odd-odd N = Z nuclei there is an enhancement of the GT strength in the low-energy region that appears to be sensitive to the T = 0 pn interaction [3]. The competition between the isovector and isoscalar pairing in odd-odd nuclei has also been discussed extensively in relation to the odd-even mass difference along the N = Z line [4,5].

On the theoretical side, the role of *pn* pairing in odd–odd N = Z nuclei is still not clear. A fair description of low-lying states and GT transitions in odd–odd N = Z nuclei is given by the shell model (SM) calculations (see, e.g., Ref. [6]). However, due to the complicated structure of the SM wavefunction, from these calculations it is not easy to draw conclusions on the role played by the *pn* pairing. Recently, the effect of T = 0 and T = 1 pairing forces on the spectroscopic properties of odd–odd N = Z nuclei was analyzed in the framework of a simple three-body model in which the odd *pn* pair is supposed to move on the top of a closed even–even core [7]. This model gives good

This is an Open Access article distributed under the terms of the Creative Commons Attribution License (http://creativecommons.org/licenses/by/4.0/),

by guest on 03 October 2017

which permits unrestricted reuse, distribution, and reproduction in any medium, provided the original work is properly cited. Downloaded from https://academic.oup.com/ptep/article-abstract/2017/7/073D05/4056193/Isovector-and-isoscalar-pairing-in-odd-odd-N-Z

results for nuclei in which the core can be considered inert, such as <sup>18</sup>F and <sup>42</sup>Sc, but not for nuclei in which the core degrees of freedom are important.

The difficulties mentioned above point to the need for new microscopic models that, on one hand, are able to describe reasonably well the spectroscopic properties of odd–odd N = Z nuclei, and, on the other hand, are simple enough to understand the impact of *pn* pairing correlations on physical observables. As an alternative, in this article we shall use the framework of the quartet condensation model (QCM) that we proposed in Ref. [8]. Its advantage is the explicit treatment of the pairing correlations in the wavefunction and, compared to other pairing models, the exact conservation of particle number and isospin. The scope of this study is to extend the QCM approach of Ref. [8], applied previously to even–even nuclei, to the case of odd–odd N = Z nuclei and to study, for these nuclei, the role played by proton–neutron pairing in the lowest T = 0 and T = 1 states.

### 2. Formalism

In the present study the isovector and isoscalar pairing correlations in odd–odd N = Z nuclei are described by pairing forces that act on pairs of nucleons moving in time-reversed single-particle states generated by axially deformed mean fields. The corresponding Hamiltonian is given by

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

In the first term  $\varepsilon_{i\tau}$  are the single-particle energies for the neutrons  $(\tau = 1/2)$  and protons  $(\tau = -1/2)$  while  $N_{i\tau}$  are the particle number operators. The second term is the isovector pairing interaction expressed by the pair operators  $P_{i,0}^+ = (v_i^+ \pi_{\bar{i}}^+ + \pi_i^+ v_{\bar{i}}^+)/\sqrt{2}$ ,  $P_{i,1}^+ = v_i^+ v_{\bar{i}}^+$  and  $P_{i,-1}^+ = \pi_i^+ \pi_{\bar{i}}^+$ , where  $v_i^+$  and  $\pi_i^+$  are creation operators for neutrons and protons in the state *i*. The last term is the isoscalar pairing interaction represented by the operators  $D_{i,0}^+ = (v_i^+ \pi_{\bar{i}}^+ - \pi_i^+ v_{\bar{i}}^+)/\sqrt{2}$ , which creates a noncollective isoscalar pair in the time-reversed states  $(i, \bar{i})$ . In the applications considered in the present paper the single-particle states have axial symmetry.

The Hamiltonian (1) was employed recently to study the isovector and isoscalar pairing correlations in even–even N = Z nuclei in the framework of the QCM approach [8]. This approach is extended here for the case of odd–odd nuclei. For reasons of consistency we start by presenting briefly the QCM approach for even–even nuclei.

In the QCM approach the ground state of the Hamiltonian (1) for a system of N neutrons and Z protons, with N = Z = even, moving above a closed core  $|0\rangle$  is described by the ansatz

$$|\text{QCM}\rangle = (A^+ + (\Delta_0^+)^2)^{n_q} |0\rangle,$$
 (2)

where  $n_q = (N + Z)/4$ . The operator  $A^+$  is the collective quartet defined by a superposition of two noncollective isovector pairs coupled to the total isospin T = 0 and has the expression

$$A^{+} = \sum_{i,j} x_{ij} [P_i^{+} P_j^{+}]^{T=0}.$$
(3)

Supposing that the mixing amplitudes  $x_{ij}$  are separable, i.e.,  $x_{ij} = x_i x_j$ , the collective quartet gets the form

$$A^{+} = 2\Gamma_{1}^{+}\Gamma_{-1}^{+} - (\Gamma_{0}^{+})^{2}, \qquad (4)$$

where  $\Gamma_t^+ = \sum_i x_i P_{i,t}^+$  are the collective neutron–neutron (t = 1), proton–proton (t = -1), and proton–neutron (t = 0) isovector pairs. Finally, in Eq. (2) the operator  $\Delta_0^+$  is the collective isoscalar pair defined by

$$\Delta_0^+ = \sum_i y_i D_{i,0}^+.$$
 (5)

When the single-particle states are degenerate and the strengths of the two pairing forces are equal, the QCM state (2) is the exact solution of the Hamiltonian (1). For realistic single-particle spectra and realistic pairing interactions the QCM state (2) is no longer the exact solution but, as shown in Ref. [8], it predicts with high accuracy the pairing correlations in even–even N = Z nuclei.

In what follows we extend the QCM approach to odd–odd N = Z systems. The main assumption, suggested by the exact solution of the Hamiltonian (1) (see below), is that the lowest T = 1 and T = 0 states in odd–odd nuclei can be well described variationally by trial states obtained by appending to the QCM function (2) a proton–neutron pair. Since the isospin of the QCM state (2) is T = 0, the total isospin of the odd–odd system is given by the isospin of the appended pair. Thus, the ansatz for the lowest T = 1 state of odd–odd N = Z systems is

$$|iv; \text{QCM}\rangle = \tilde{\Gamma}_0^+ (A^+ + (\Delta_0^+)^2)^{n_q} |0\rangle, \tag{6}$$

where  $\tilde{\Gamma}_0^+ = \sum_i z_i P_{i,0}^+$  is the isovector *pn* pair attached to the even–even part of the state (in what follows we shall use the name "core" for the even–even part of the state (6), which should not be confused with the closed core  $|0\rangle$ ). It can be seen that this pair has a different collectivity compared to the isovector *pn* pair  $\Gamma_0^+$  contained in the quartet  $A^+$  (see Eq. 4).

Likewise, the lowest T = 0 state of odd-odd N = Z systems is described by the function

$$|is; \text{QCM}\rangle = \tilde{\Delta}_{0}^{+} (A^{+} + (\Delta_{0}^{+})^{2})^{n_{q}} |0\rangle,$$
 (7)

where  $\tilde{\Delta}_0^+ = \sum_i z_i D_{i,0}^+$  is the odd isoscalar pair, which also has a different structure compared to the isoscalar pair  $\Delta_0^+$ , which enters in the even–even core. Due to its different isospin, the state (7) is orthogonal to the isovector state (6).

We have proved that the states (6), (7) are exact eigenfunctions of the Hamiltonian (1) when the single-particle energies are degenerate and when the pairing forces have the same strength, i.e.,  $V^{T=1}(i,j) = V^{T=0}(i,j) = g$ . In this case the states (6), (7) have the same energy, which, for  $\epsilon_i = 0$ , is given by

$$E(n_q, v) = (v - 2n_q)g + 2n_q(v - n_q + 2)g,$$
(8)

where  $n_q$  is the number of quartets and  $\nu$  is the number of single-particle levels. In Eq. (8) the second term corresponds to the energy of the even-even core of the functions (6), (7). It is worth mentioning that this exact solution is not the exact solution of the SU(4) model [9] because in the Hamiltonian (1) the isoscalar force contains only pairs in time-reversed single-particle states.

For a nondegenerate single-particle spectrum and general pairing forces the QCM states (6), (7) are determined variationally. The variational parameters are the amplitudes  $x_i$ ,  $y_i$ , and  $z_i$  that define, respectively, the isovector pairs  $\Gamma_t^+$ , the isoscalar pair  $\Delta_0^+$ , and the odd *pn* pair. They are found by minimizing the average of the Hamiltonian (1) on the QCM states (6), (7) and by imposing, for the latter, a normalization condition. The average of the Hamiltonian and the norm of the QCM states are

calculated using the technique of recurrence relations. More precisely, the calculations are performed using auxiliary states composed of products of collective pairs. Thus, for the isovector T = 1 state (6) the auxiliary states are

$$|n_1 n_2 n_3 n_4 n_5\rangle = (\Gamma_1^+)^{n_1} (\Gamma_{-1}^+)^{n_2} (\Gamma_0^+)^{n_3} (\Delta_0^+)^{n_4} (\tilde{\Gamma}_0^+)^{n_5} |0\rangle.$$
(9)

The auxiliary states for the calculations of the isoscalar T = 0 state (7) have a similar structure with the difference that the odd isovector pair  $\tilde{\Gamma}_0^+$  is replaced by the odd isoscalar pair  $\tilde{\Delta}_0^+$ . It can be observed that the QCM states (6), (7) can be expressed in terms of a subset of auxiliary states corresponding to specific combinations of  $n_i$ . However, in order to close the recurrence relations one needs to evaluate the matrix elements of the Hamiltonian (1) for all auxiliary states that satisfy the conditions  $\sum_i n_i = (N + Z)/2$  and  $n_5 = 0, 1$ . An example of recurrence relations, for the case of even-even systems, can be seen in Refs. [10,11].

The advantage of the QCM approach is the possibility of direct investigation of the role of various types of correlations by simply switching them on and off in the structure of the states (6), (7). Thus, in order to explore the importance of isoscalar pairing on the lowest T = 0 and T = 1 states in odd–odd N = Z systems, one can remove the isoscalar pair  $\Delta_0^+$  from the functions (6), (7). In this approximation the functions get the expressions

$$|is;Q_{i\nu}\rangle = \tilde{\Delta}_0^+ (A^+)^{n_q} |0\rangle, \tag{10}$$

$$|iv;Q_{iv}\rangle = \tilde{\Gamma}_0^+ (A^+)^{n_q} |0\rangle.$$
<sup>(11)</sup>

Alternatively, we can estimate the importance of the isovector pairing by removing the isovector quartet  $A^+$  from the QCM functions. The corresponding functions are

$$|C_{is}\rangle = (\Delta_0^+)^{2n_q+1}|0\rangle,$$
 (12)

$$|iv; C_{is}\rangle = \tilde{\Gamma}_0^+ (\Delta_0^{+2})^{n_q} |0\rangle.$$
<sup>(13)</sup>

Another possibility is to remove the contribution of like-particle pairs from the QCM functions, keeping only the isovector and isoscalar pn pairs. These trial states, which can be employed to study the role of like-particle pairing in N = Z nuclei, have the expressions

$$|is; C_{iv}\rangle = \tilde{\Delta}_0^+ (\Gamma_0^{+2})^{n_q} |0\rangle, \tag{14}$$

$$|C_{iv}\rangle = (\Gamma_0^+)^{2n_q+1}|0\rangle.$$
(15)

In contrast to the previous approximations, the states (14), (15) do not have a well defined isospin.

Among the approximations mentioned above, of special interest are the ones corresponding to the states (12) and (15), which are pure condensates of isoscalar and isovector pn pairs, respectively. These states are sometimes considered as representative for understanding the competition between isovector and isoscalar proton–neutron pairing in nuclei.

The QCM states (6), (7) and all the approximations based on them are formulated here in the intrinsic system associated with the axially deformed single-particle levels. Therefore, they have a well defined projection of the angular momentum on the *z*-axis but not a well defined angular momentum. A more complicated quartet formalism for odd–odd nuclei, which exactly conserves the angular momentum and takes into account the correlations induced by a general two-body force, was recently proposed in Ref. [12].

## 3. Results

To test the accuracy of the QCM approach for odd–odd N = Z nuclei we consider nuclei with protons and neutrons outside the closed <sup>16</sup>O, <sup>40</sup>Ca, and <sup>100</sup>Sn cores. To perform the calculations, we use a similar input for the pairing forces and single-particle states as in our previous study on even–even nuclei [8]. Thus, the single-particle states are generated by axially deformed mean fields calculated with the Skyrme–HF code *ev8* [13] and with the force *Sly4* [14]. In the mean-field calculations the Coulomb interaction is switched off, so the single-particle energies for protons and neutrons are the same.

The single-particle energies and the pairing matrix elements used as inputs in the QCM calculations of odd–odd N = Z nuclei are extracted from the even–even (N - 1, Z - 1) nuclei. For <sup>30</sup>P we use the mean field of the nucleus (N + 1, Z + 1) instead, i.e., <sup>32</sup>S, which provides a better description of the energy difference between the first excited state and the ground state. The deformations predicted by the mean-field calculations for the even–even N = Z nuclei employed in the present calculations are displayed in Table 1. They are defined as

$$\beta_{\rm th} = \left(\frac{5\pi}{9}\right)^{\frac{1}{2}} \frac{\langle \hat{Q}_2 \rangle}{AR_0^2},\tag{16}$$

where A is the mass number,  $R_0 = 1.2A^{\frac{1}{3}}$ , and  $\hat{Q}_2$  is the quadrupole operator. It can be observed that in the sd and pf-shell nuclei the calculated deformations follow the experimental values reasonably well, except for <sup>32</sup>S, which is spherical in mean-field calculations. We have, however, checked that the results for <sup>30</sup>P discussed below do not change significantly if we use a deformed mean field for <sup>32</sup>S as input in the QCM calculations.

For pairing forces we use a zero-range delta interaction  $V^T(r_1, r_2) = V_0^T \delta(r_1 - r_2) \hat{P}_{S,S_z}^T$ , where  $\hat{P}_{S,S_z}^T$  is the projection operator on the spin of the pairs, i.e., S = 0 for the isovector (T = 1) force and  $S = 1, S_z = 0$  for the isoscalar (T = 0) force. The matrix elements of the pairing forces are calculated using the single-particle wavefunctions generated by the Skyrme–HF calculations (for details, see Ref. [15]). As parameters we use the strength of the isovector force, denoted by  $V_0$ , and the scaling factor w that defines the strength of the isoscalar force,  $V_0^{T=0} = wV_0$ . Determining how to fix these parameters is not a simple task. Since the main goal of this study is to test the accuracy of the QCM approach, we have made several calculations, from the weak to the strong pairing regime. Because the conclusions relevant to this study are quite similar for all these strengths, here we present only the results for the pairing strength  $V_0 = 465$  MeV fm<sup>-3</sup> employed in our previous study of even–even nuclei [8]. The pairing interaction is of zero range and therefore the results of the calculations depend not only on the pairing strength but also on the size of the model space. All the QCM results presented in this study correspond to calculations done in a model space composed of the first 10 single-particle states above the closed <sup>16</sup>O, <sup>40</sup>Ca, and <sup>100</sup>Sn cores.

**Table 1.** Theoretical ( $\beta_{th}$ ) versus experimental ( $\beta_{exp}$ ) quadrupole deformations of even–even N = Z nuclei, from which are extracted the single-particle energies and pairing matrix elements employed in the QCM calculations of odd–odd nuclei listed in Table 2. The experimental data are from Ref. [16].

	<sup>20</sup> Ne	<sup>24</sup> Mg	<sup>32</sup> S	<sup>44</sup> Ti	<sup>48</sup> Cr	<sup>52</sup> Fe	<sup>104</sup> Te	<sup>108</sup> Xe	<sup>112</sup> Ba
$\beta_{ m th}$	0.497	0.488	0.000	0.188	0.290	0.233	0.113	0.119	0.001
$eta_{ ext{exp}}$	0.720	0.613	0.314	0.260	0.368	0.230	_	_	—

Downloaded from https://academic.oup.com/ptep/article-abstract/2017/7/073D05/4056193/Isovector-and-isoscalar-pairing-in-odd-odd-N-Z by guest on 03 October 2017



Fig. 1. The energy difference between the lowest T = 1 and T = 0 states as a function of N = Z = A/2. The experimental data are extracted from Ref. [16]. The solid lines show the exact results obtained by diagonalizing the Hamiltonian (1). The calculations correspond to the strength  $V_0 = 465$  MeV fm<sup>-3</sup> and to various scaling factors w.

For the scaling factor w we also used various values,  $w = \{1.0, 1.3, 1.5, 1.6\}$ . To find the most appropriate value of w for the strength  $V_0 = 465 \text{ MeV fm}^{-3}$  we searched for the best agreement with the energy difference between the first excited state and the ground state of odd-odd nuclei. These energy differences are shown in Fig. 1 by black squares. It is worth mentioning that the lowest T = 0 state can have various angular momenta  $J \ge 1$  (e.g., the ground states of <sup>22</sup>Na and <sup>26</sup>Al have J = 3 and J = 5, respectively).

The theoretical results shown in Fig. 1 correspond to the exact diagonalization of the Hamiltonian (1) in a space spanned by 10 single-particle levels above the <sup>16</sup>O and <sup>40</sup>Ca cores. The best agreement with the experimental data is obtained by choosing w = 1.6 for *sd*-shell nuclei and w = 1.0 for *pf*-shell nuclei. The results corresponding to this choice are indicated in Fig. 1 by full symbols. In Fig. 1 we also show the results obtained considering only the isovector pairing force, i.e., for w = 0.0. It can be seen that in this case the predictions are quite far from the data, especially for the *sd*-shell nuclei. For the nuclei above <sup>100</sup>Sn there are no experimental data on low-lying states available to be used for fixing the scaling factor *w*. Therefore, for these nuclei, we have chosen the same value for *w* as for the *pf*-shell nuclei.

With the parameters of the Hamiltonian fixed as explained above, we have studied the accuracy of the energies of the lowest T = 0 and T = 1 states predicted by the extended QCM approach for the odd-odd nuclei. The results are presented in Table 2. This shows the correlation energies defined as  $E_{\text{corr}} = E_0 - E$ , where E is the total energy, while  $E_0$  is the noninteracting energy obtained by switching off the pairing interactions. The correlation energies predicted by the QCM functions (6), (7) are given in the fourth column. The errors relative to the exact energies shown in the third column are given in brackets. It can be observed that, for all the states and nuclei shown in Table 2, the errors are small, under 1%. We can thus conclude that the QCM functions (6), (7) provide an accurate description of the lowest T = 0 and T = 1 states of the Hamiltonian (1).

One of the advantages of the QCM approach is the opportunity to study the relevance of various types of pairing correlations directly through the structure of the trial states (6), (7). As discussed in the previous section, this is possible by using the approximations (10)–(15). The correlation energies corresponding to these approximations are shown in Table 2. The errors relative to the exact results are given in brackets. One can observe that the smallest errors correspond to the approximations (10), (11), in which the contribution of the isoscalar pairs in the even–even core of the QCM functions is

			• • • •	<b>`</b>		
		Exact	QCM>	$ iv/is; QCM_{iv}\rangle$	$ iv;C_{is} angle/ C_{is} angle$	$ C_{iv}\rangle/ is;C_{iv}\rangle$
<sup>22</sup> Na	T = 0	13.87	13.87 (0.00%)	13.86 (0.07%)	13.85 (0.12%)	13.85 (0.15%)
	T = 1	13.23	13.23 (0.03%)	13.22 (0.05%)	12.97 (1.97%)	13.22 (0.11%)
<sup>26</sup> Al	T = 0	22.06	22.05 (0.03%)	22.04 (0.07%)	21.94 (0.53%)	21.79 (1.24%)
	T = 1	21.07	21.06 (0.02%)	21.05 (0.07%)	20.93 (0.66%)	20.98 (0.41%)
<sup>30</sup> P	T = 0	12.66	12.60 (0.44%)	12.55 (0.86%)	11.96 (5.86%)	11.94 (5.95%)
	T = 1	11.72	11.66 (0.44%)	11.62 (0.82%)	10.94 (7.11%)	10.96 (6.94%)
<sup>46</sup> V	T = 1	7.92	7.92 (0.04%)	7.91 (0.10%)	7.33 (8.11%)	7.76 (2.11%)
	T = 0	6.93	6.93 (0.01%)	6.93 (0.07%)	6.73 (2.99%)	6.79 (2.05%)
<sup>50</sup> Mn	T = 1	12.77	12.76 (0.07%)	12.75 (0.14%)	12.52 (2.02%)	12.62 (1.22%)
	T = 0	12.37	12.36 (0.04%)	12.34 (0.24%)	12.18 (1.61%)	12.19 (1.48%)
<sup>54</sup> Co	T = 1	16.14	16.12 (0.14%)	16.09 (0.28%)	15.67 (3.01%)	15.86 (1.78%)
	T = 0	15.93	15.92 (0.04%)	15.89 (0.22%)	15.53 (2.56%)	15.66 (1.73%)
$^{106}I$	T = 1	5.15	5.14 (0.08%)	5.13 (0.23%)	4.71 (9.37%)	4.93 (4.51%)
	T = 0	4.53	4.52 (0.04%)	4.51 (0.42%)	4.19 (7.84%)	4.29 (5.53%)
$^{110}Cs$	T = 1	8.03	7.98 (0.56%)	7.97 (0.75%)	7.16 (12.14%)	7.59 (5.86%)
	T = 0	7.09	7.06 (0.45%)	7.04 (0.80%)	6.47 (9.64%)	6.65 (6.77%)
<sup>114</sup> La	T = 1	9.76	9.72 (0.36%)	9.69 (0.73%)	8.79 (11.03%)	9.27 (5.23%)
	T = 0	8.95	8.93 (0.28%)	8.92 (0.42%)	8.31 (7.74%)	8.51 (5.18%)

**Table 2.** Correlation energies, in MeV, for the lowest T = 1 and T = 0 states. The errors relative to the exact values indicated in the third column are given in brackets. The results corresponding to the QCM states (6), (7) and to the approximations defined by Eqs. (10)–(15) are shown.

neglected. It can be seen that, compared to the calculations with the full QCM functions, the errors in these approximations are increased 2–3 times for the T = 1 states and by larger factors for some T = 0 states. However, all the errors relative to the exact results remain under 1%.

In the sixth column are shown the results corresponding to the approximations (12), (13), in which the isovector quartet is taken out from the even-even core. We can see that in this case the errors are much bigger than in the case in which the isoscalar pairs are neglected. In the last column are given the results of approximations (14), (15), obtained by neglecting the contribution of like-particle pairs in the QCM states. It can be noticed that, for all nuclei, the states T = 1 are better described by a condensate of isovector *pn* pairs rather than by the approximation (13). On the other hand, the ground T = 0 states of *sd*-shell nuclei are slightly better described by a condensate of solvector *T* = 0 states of *sd*-shell nuclei are slightly better described by a condensate of isoscalar *pn* pairs rather than the approximation (14). However, the latter approximation is far better than the former in the case of excited T = 0 states of *pf*-shell nuclei and nuclei with A > 100.

Overall, these calculations show that the T = 0 and T = 1 states cannot be well described as pure condensates of isoscalar and isovector pairs, respectively. In general, neglecting the contribution of like-particle pairs generates large errors. The best approximation, for both T = 0 and T = 1 states, is the one in which the odd *pn* pair is appended to a condensate of isovector quartets. This fact indicates that the 4-body quartet correlations play an important role in odd–odd N = Z nuclei. As demonstrated in Ref. [10], these correlations are missed when the condensate of isovector quartets is replaced by products of pair condensates.

To better understand how the different pairing modes contribute to the total energy, in Fig. 2 are shown the isovector and isoscalar pairing energies for the ground states of *sd* and *pf* nuclei. The pairing energies are calculated by averaging the corresponding pairing forces on the QCM functions (6), (7). It is important to observe that the pairing energies for T = 1 (T = 0) states also include



Fig. 2. Pairing energies, in MeV, for the odd–odd N = Z nuclei as a function of the mass number A. In the upper (lower) panel are shown the results for the sd-shell (pf-shell) nuclei.

contributions from the isoscalar (isovector) pairing correlations, a fact that comes from the mixing of isovector and isoscalar degrees of freedom through the even–even core of the QCM functions.

In the upper (a) panel of Fig. 2 are plotted the pairing energies in the ground T = 0 states of *sd*-shell nuclei. The pairing energy  $E_{pn}^{T=0}$  for <sup>18</sup>F, which corresponds to one T = 0 pair above <sup>16</sup>O, is shown for reference. It can be seen that the curves for  $E_{pn}^{T=0}$  and  $E_{pn}^{T=1}$  are almost parallel. This indicates that the extra pairing energy in the T = 0 channel for A > 18 is related mainly to the contribution of the odd *pn* T = 0 pairs. It is also worth noticing that the total pairing energy in the T = 1 channel also contains the contribution from the proton–proton (*pp*) and neutron–neutron (*nn*) pairing energies, which, due to the isospin symmetry, are equal to the *pn* T = 1 pairing energy. Therefore, the total isovector pairing energy is comparable to the isoscalar pairing energy, although the latter contains in addition a large contribution from the extra odd T = 0 pair.

In the lower (b) panel of Fig. 2 are plotted the pairing energies for the T = 1 ground states of *pf*-shell nuclei. It can be seen that  $E_{pn}^{T=0}$  is smaller than  $E_{pn}^{T=1}$  and also smaller than the like-particle pairing energy. At variance with what is seen in the upper panel, the energy difference  $E_{pn}^{T=1} - E_{pn}^{T=0}$  for A > 42 is much larger than the energy of the odd *pn* T = 1 pair in <sup>42</sup>Sc. Therefore, the larger *pn* pairing energy in the isovector channel is not caused only by the extra *pn* T = 1 pair attached to the even–even core.

			1				0					
-	<sup>26</sup> A1		<sup>26</sup> Al <sup>30</sup> P		<sup>50</sup> Mn		<sup>54</sup> Co		$^{110}Cs$		<sup>114</sup> La	
	T = 1	T = 0	T = 1	T = 0	T = 1	T = 0	T = 1	T = 0	T = 1	T = 0	T = 1	T = 0
$K_x$	1.25	1.92	3.05	3.05	1.47	1.41	2.37	2.36	1.64	1.66	3.18	3.09
$K_{v}$	1.97	1.31	1.89	1.56	2.39	1.33	1.72	1.25	2.24	1.88	1.16	1.24
Κ <sub>z</sub>	2.77	1.63	2.82	1.65	1.99	1.09	2.30	1.63	2.34	1.29	4.09	1.33

**Table 3.** Schmidt numbers for the proton-neutron pairs in the lowest T = 1 and T = 0 states of various odd-odd N = Z nuclei.  $K_x$  and  $K_y$  denote the Schmidt numbers for the pairs  $\Gamma_0^+$  and  $\Delta_0^+$  while  $K_z$  is the Schmidt number for the odd pair, i.e.,  $\tilde{\Gamma}_0^+$  for T = 1 states and  $\tilde{\Delta}_0^+$  for T = 0 states.

The T = 0 states in odd-odd N = Z nuclei are often described as states having a two-quasiparticle structure. Thus, to evaluate the energies of T = 0 states, the blocking procedure is commonly employed, in which the odd T = 0 pair is not considered as a collective pair in which the nucleons are scattered on nearby single-particle levels but just as a proton and a neutron sitting on a single level. In what follows we are going to examine the validity of this approximation in the framework of the QCM approach. In order to analyze this issue, we need a working definition for the collectivity of a pair. Here we shall use the so-called Schmidt number, which is commonly employed to analyze the entanglement of composite systems formed by two parts [17]. In the case of a pair operator  $\Gamma^+ = \sum_{i=1}^{n_s} w_i a_i^+ a_i^+$ , the Schmidt number has the expression  $K = (\sum_i \omega_i^2)^2 / \sum_i \omega_i^4$  (for an application of K to like-particle pairing, see Ref. [18]). When there is no entanglement, K = 1, while, when the entanglement is maximum, which means equal occupancy of all available states,  $K = n_s$ , where  $n_s$  is the number of states. As examples, in Table 3 we show for some nuclei the Schmidt numbers corresponding to the pairs that compose the QCM states (6), (7). In Table 3,  $K_x$ and  $K_y$  denote the Schmidt numbers associated with the isovector pair  $\Gamma_0^+$  and the isoscalar pair  $\Delta_0^+$ , respectively. Since in the isovector quartet  $A^+$  all the isovector pairs have the same structure, the like-particle pairs have the Schmidt number  $K_x$ , like the isovector pn pair.  $K_z$  denotes the Schmidt number for the odd pair, i.e.,  $\tilde{\Gamma}_0^+$  for the T = 1 state and  $\tilde{\Delta}_0^+$  for the T = 0 state. We recall that the T = 0 state is the ground state for <sup>30</sup>P and the excited state for <sup>54</sup>Co and <sup>114</sup>La. All pairs are spread on a maximum of  $n_s = 10$  states.

From Table 3 it can be observed that the T = 0 pairs are less collective than the isovector T = 1 pairs, which is in agreement with the stronger T = 1 pairing correlations emerging from the results shown in Table 2. In particular, the odd T = 0 pair is less collective than the odd T = 1 pair. However, in all nuclei, except <sup>50</sup>Mn, the collectivity of the odd T = 0 pair is significant and comparable to the collectivity of the T = 0 pairs in the even–even core of the QCM states. Therefore, these calculations indicate that, in general, the T = 0 states do not have a pure two-quasiparticle character.

#### 4. Summary

In this paper we have studied the role of isovector and isoscalar pairing correlations in the lowest T = 1 and T = 0 states of odd-odd N = Z nuclei. This study is performed in the framework of the QCM approach, which was extended from even-even to odd-odd nuclei. In the extended QCM formalism the lowest T = 0 and T = 1 states of odd-odd self-conjugate nuclei are described by a condensate of quartets to which is appended an isoscalar or an isovector proton-neutron pair. As in Ref. [8], the quartets are taken as a linear superposition of an isovector quartet and two collective isoscalar pairs. This model was tested for realistic pairing Hamiltonians and for nuclei with valence nucleons moving above the cores <sup>16</sup>O, <sup>40</sup>Ca, and <sup>100</sup>Sn. A comparison with exact results shows

that the energies of the lowest T = 1 and T = 0 states can be described with high precision by the QCM approach. Taking advantage of the structure of the QCM functions, we then analyzed the competition between the isovector and isoscalar pairing correlations and the accuracy of various approximations. This analysis indicates that, in the nuclei mentioned above, the isoscalar pairing correlations are weaker but they coexist with the isovector correlations in both the T = 0 and T = 1states. To describe these states accurately is essential to include the isovector pairing through the isovector quartets, in which the isovector pn pairs are coupled together to like-particle pairs. Any approximations in which the contribution of the like-particle pairing is neglected, including those in which the T = 1 and T = 0 states are described by a condensate of isovector pn pairs and of isoscalar pn pairs, respectively, do not accurately describe the pairing correlations in odd-odd N = Z nuclei.

In the present study, the lowest T = 0 and T = 1 states are calculated in the intrinsic system of the axially deformed mean field and therefore they do not have a well defined angular momentum. The restoration of angular momentum will be treated in a future study.

#### Acknowledgements

N.S. is grateful for the hospitality of IPN-Orsay, Université Paris-Sud, where this paper was written. This work was supported by the Romanian National Authority for Scientific Research through the grants 5/5.2/FAIR-RO and PN 16420101/2016. D.N. acknowledges the support of the French Embassy and French Institute in Romania through a three month post-doc fellowship.

## References

- [1] S. Frauendorf and A. O. Macchiavelli, Prog. Part. Nucl. Phys. 78, 24 (2014).
- [2] H. Sagawa, C. L. Bai, and G. Colò, Phys. Scripta 91, 083011 (2016).
- [3] Y. Fujita et al., Phys. Rev. Lett. 112, 112502 (2014).
- [4] A. O. Macchiavelli et al., Phys. Rev. C 61, 041303(R) (2000).
- [5] P. Vogel, Nucl. Phys. A 662, 148 (2000).
- [6] M. Honma, T. Otsuka, B. A. Brown and T. Mizusaki, Phys. Rev. C 69, 034335 (2004).
- [7] Y. Tanimura, H. Sagawa, and K. Hagino, Prog. Theor. Exp. Phys. 2014, 053D02 (2014).
- [8] N. Sandulescu, D. Negrea, and D. Gambacurta, Phys. Lett. B 751, 348 (2015).
- [9] J. Dobes and S. Pittel, Phys. Rev. C 57, 688 (1998).
- [10] N. Sandulescu, D. Negrea, J. Dukelsky, and C. W. Johnson, Phys. Rev. C 85, 061303(R) (2012).
- [11] D. Negrea, Proton-neutron pairing correlations in atomic nuclei, *Ph.D. Thesis*, University of Bucharest and Université Paris-Sud (2013). (Available at: https://tel.archives-ouvertes.fr/tel-00870588/document.)
- [12] M. Sambataro and N. Sandulescu, Phys. Lett. B 763, 151 (2016).
- [13] P. Bonche, H. Flocard, and P. Heenen, Comput. Phys. Commun. 171, 49 (2005).
- [14] E. Chabanat, P. Bonche, P. Haensel, J. Meyer and R. Schaeffer, Nucl. Phys. A 627, 710 (1997).
- [15] D. Gambacurta and D. Lacroix, Phys. Rev. C 91, 014308 (2015).
- [16] National Nuclear Data Center, Brookhaven National Laboratory. (Available at: http://www.nndc.bnl.gov.)
- [17] C. K. Law, Phys. Rev. A 71, 034306 (2005).
- [18] N. Sandulescu and G. F. Bertsch, Phys. Rev. C 78, 064318 (2008).