Proton-neutron pairing and binding energies of nuclei close to 
\( N=Z \) line

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Abstract

We analyse the contribution of isovector and isoscalar proton-neutron pairing to the binding energies of even-even nuclei with \( N-Z = 0,2,4 \) and atomic mass \( 20 < A < 100 \). The binding energies are calculated in the mean-field approach by coupling a Skyrme-type functional to an isovector-isoscalar pairing force of zero range. The latter is treated in the framework of quartet condensation model (QCM), which conserves exactly the particle number and the isospin. The interdependence of pairing and deformation is taken into account by performing self-consistent Skyrme-HF+QCM calculations in the intrinsic system. It is shown that the binding energies are not changing much when the isoscalar pairing is switched on. This fact is related to the off-diagonal matrix elements of the pairing force, which is less attractive for the isoscalar force, and to the competition between the isoscalar and isovector pairing channels.

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I. INTRODUCTION

In nuclei close to $N = Z$ line, it is usually considered to be important two types of proton-neutron (pn) pairing correlations, corresponding to spin-singlet isovector ($S=0,T=1$) and spin-triplet isoscalar ($S=1,T=0$) pn pairs. Due to the isospin invariance of nuclear forces, the isovector pn pairing is supposed to play a similar role as the standard neutron-neutron and proton-proton pairing. Much less it is known however about the role played by the isoscalar pn pairing in nuclei. In fact, for quite many years, a lot of efforts have been focused on finding the fingerprints of isoscalar pn pairing correlations in various nuclear observables such as binding energies, high-spin excitations, proton-neutron transfer cross sections, etc. (e.g., see the recent reviews [1, 2]).

The majority of theoretical studies on pn pairing have been done in the Hartree-Fock-Bogoliubov (HFB) approach. In HFB the pn pairing, both isovector and isoscalar, is treated together with the like-particle pairing through the generalized Bogoliubov transformation (e.g., see [3–5] and the references quoted therein). For most of nuclei, the HFB calculations predict $T=1$ pairing correlations in the ground state. The $T=0$ pairing and the coexistence between $T=1$ and $T=0$ pairing is predicted for a few nuclei, but these predictions depend strongly on the chosen parameters and the calculation scheme. It is also not clear how these predictions are affected by the non-conservation of particle number, the isospin and the angular momentum, which are specific to the HFB calculations done with the isovector-isoscalar pairing interactions. To conserve all these quantities in HFB calculations is a difficult task and some results on this line exist only for the trivial case of degenerate levels [6, 7]. Realistic beyond-HFB calculations with particle number and angular momentum projections have been done recently, but with the projection performed after the variation [8]. Another source of uncertainty comes from the fact that in the majority of HFB calculations the mean field is kept fixed, so it is not taken into account dynamically the competition between pairing and deformation [4]. This is also the case of the most recent HFB calculations, done on the top of a fixed spherically-symmetric mean field, in which the effect of the deformation on pairing is neglected completely [5].

An alternative approach to take into account the isovector-isoscalar pairing correlations in mean-field approximations was proposed in Refs [9, 10]. In this approach, called Quartet Condensation Model (QCM), the ground state of $N=Z$ nuclei is described as a product
of quartets built by two protons and two neutrons coupled to the total isospin \( T=0 \). By construction, in QCM the ground state is conserving exactly both the particle number and the isospin. When the quartets are built with spherically symmetric single-particle states, the QCM ground state has also a well-defined angular momentum [11].

Previous studies have shown that the QCM approach provides accurate results for isovector-isoscalar pairing Hamiltonians which can be solved exactly [9–11]. The purpose of this work is to extend these studies to self-consistent mean-field plus pairing calculations and to analyse, within the QCM framework, the contribution of \( T=1 \) and \( T=0 \) pairing correlations to the ground state energy of nuclei close to \( N=Z \) line. The novel feature of the present calculations is that they take into account dynamically the competition between pairing and deformation in a formalism which conserves exactly both the particle number and the isospin.

II. THE FORMALISM

To calculate the binding energies, we use a self-consistent mean-field plus pairing formalism. The calculations are done in the intrinsic system defined by an axially deformed mean-field generated by a Skyrme functional. The pairing correlations are induced by an isovector-isoscalar pairing force which scatters pairs of nucleons in time-reversed states. To evaluate the contribution of pairing correlations to the binding energies, we employ the QCM approach introduced in Refs [9, 10]. For the sake of completeness, the QCM formalism is shortly presented below.

The isovector and isoscalar pairing correlations are calculated for a set of axially-deformed single-particle states. They are described by the Hamiltonian [9],

\[
H = \sum_{i,\tau=\pm 1/2} \varepsilon_{i,\tau} N_{i,\tau} + \sum_{i,j} V_{i,j}^{(T=1)} \sum_{t=-1,0,1} P_{i,t}^\dagger P_{j,t} + \sum_{i,j} V_{i,j}^{(T=0)} D_{i,0}^\dagger D_{j,0},
\]

where \( \varepsilon_{i,\tau} \) are the single-particle energies of 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 isovector pair operators \( P_{i,1}^\dagger = \nu_i^\dagger \nu_i^\dagger \), \( P_{i,-1}^\dagger = \pi_i^\dagger \pi_i^\dagger \), \( P_{i,0}^\dagger = (\nu_i^\dagger \pi_i^\dagger + \pi_i^\dagger \nu_i^\dagger)/\sqrt{2} \). The third term is the isoscalar pairing interaction and \( D_{i,0}^\dagger = (\nu_i^\dagger \pi_i^\dagger - \pi_i^\dagger \nu_i^\dagger)/\sqrt{2} \) is the isoscalar
pair operator. By $\nu^\dagger_i$ and $\pi^\dagger_i$ are denoted the creation operators for neutrons and protons in the state $i$, while $\tilde{i}$ is the time conjugate of the state $i$. The states $i$, which correspond to the axially deformed mean-field, are characterised by the quantum numbers $i \equiv \{a_i, \Omega_i\}$, where $\Omega_i$ is the projection of the angular momentum on the symmetry axis.

By construction, in Eq. (1) the pairs operators have $J_z = 0$ but not a well-defined angular momentum $J$. In fact, when expressed in the laboratory frame, the isovector and the isoscalar intrinsic pairs can be written as a superposition of pairs with $J = 0, 2, 4, \ldots$ and, respectively, $J = 1, 3, 5, \ldots$. Therefore, the Hamiltonian (1) takes into account, in an effective way, pairing correlations which are not restricted only to the standard $(J=0,T=1)$ and $(J=1,T=0)$ channels.

In order to find the ground state energy of the Hamiltonian (1), we employ the quartet condensation model (QCM). Thus, according to QCM, the ground state of Hamiltonian (1) for even-even $N = Z$ systems is approximated by the trial state [9]

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

where $n_q = (N + Z)/2$, while $|0\rangle$ is the "vacuum" state represented by the nucleons which are supposed to be not affected by the pairing interaction. The operator $A^\dagger$ is the isovector quartet built by two isovector non-collective pairs coupled to the total isospin $T = 0$, i.e.,

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

Assuming that the mixing coefficients are separable, i.e., $x_{ij} = x_i x_j$, the isovector quartet takes the form

$$A^\dagger = 2\Gamma_1^\dagger \Gamma_{-1}^\dagger - (\Gamma_0^\dagger)^2, \quad (4)$$

where

$$\Gamma_t^\dagger = \sum_i x_i P_{i,t}^\dagger \quad (5)$$

are collective pair operators for neutron-neutron pairs ($t = 1$), proton-proton pairs ($t = -1$) and proton-neutron pairs ($t = 0$). The isoscalar degrees of freedom are described by the collective isoscalar pair

$$\Delta_0^\dagger = \sum_i y_i D_{i,0}^\dagger. \quad (6)$$

For even-even systems with $N > Z$ (the case $N < Z$ is treated in the same manner) the ground state is described by [10]

$$|QCM\rangle = (\tilde{\Gamma}_1^\dagger)^{n_N} (A^\dagger + \Delta_{0}^{\dagger 2})^{n_q}|0\rangle,$$

where

$$\tilde{\Gamma}_1^\dagger = \sum_i x_i \tilde{P}_i^\dagger \quad (5)$$

and

$$\tilde{P}_i^\dagger = \sum_j x_j P_{i,j}^\dagger \quad (5)$$

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For even-even systems with $N > Z$ (the case $N < Z$ is treated in the same manner) the ground state is described by [10]
where \( n_N = (N - Z)/2 \) gives the number of neutron pairs in excess, while \( n_q = (N + Z - 2n_N)/4 \) denotes the maximum number of quartets which can be formed with \( Z \) protons. As in the case of \( N = Z \) nuclei, here by \( Z \) and \( N \) are denoted the numbers of protons and neutrons above the \( N = Z \) core \( |0\rangle \), which are affected by the pairing interaction. The extra neutrons are represented by the collective neutron pair

\[
\hat{\Gamma}_1^\dagger = \sum_i z_i \hat{P}_i^\dagger.
\]

As can be seen, the structure of the extra pairs, expressed by the mixing amplitudes, is different from the structure of the neutron pairs which enter in the definition of the isovector quartet (4).

The QCM states depend on the mixing amplitudes of the collective pair operators. They are determined variationally by minimizing the average of the Hamiltonian under the normalization condition imposed to the trial state. Details about these calculations are presented in Ref. [9] and in the Appendix of Ref. [10].

The QCM calculations for the Hamiltonian (1) are performed iteratively with the Skyrme-HF calculations in a similar way as in the axially-deformed Skyrme+BCS calculations [12]. Thus, at a given iteration, the QCM equations are solved for the single-particle states generated by the Skyrme functional. Then, the occupation probabilities of the single-particle states provided by QCM are employed to get new densities and a new Skyrme functional which, in turn, is generating new single-particle states. At the convergence, the binding energy is obtained by adding to the mean-field energy the contribution of the pairing energy. The latter is calculated as the average of the pairing force from which it is extracted out the contribution of self-energy terms. For the like-particle pairing these terms are

\[
E_{n(p)}^{mf} = \sum_i V_T^{T=1}(i, i)v_{i,n(p)}^4,
\]

while for the pn pairing the expressions are

\[
E_{pn}^{mf}(T) = \sum_i V_T(i, i)v_{i,p}^2 v_{i,n}^2.
\]

In the expressions above, \( v_{i,n(p)}^2 \) are the occupation probabilities for neutrons (protons) corresponding to the states included in the pairing calculations. The terms (9,10), which would renormalize the single-particle energies generated by the Skyrme functional, are neglected.
since in the Skyrme-HF+QCM calculations the pairing force is a residual interaction acting only in the particle-particle channel.

In the present calculations, for the isovector-isoscalar pairing interaction we employ a zero range force of the form:

\[ V^T(r_1, r_2) = V^T_0 \delta(r_1 - r_2) \hat{P}_{S, S_z}^{T} \]

(11)

where \( \hat{P}_{S, S_z}^{T} \) is the projection operator on the spin of the pairs, namely, \( S = 0 \) for the isovector force and \( S = 1, S_z = 0 \) for the isoscalar force. The matrix elements of the pairing interaction (11) for the single-particle states provided by the Skyrme functional are calculated as shown in the Appendix of Ref. [13].

To distinguish between various quantities originating from the pairing interaction (11), in what follows we shall denote by interaction energy the average of the pairing interaction on the QCM state, by pairing energy the average of the pairing force without the contribution of the terms (9,10), while the average of the latter is denoted by self-energy.

III. RESULTS

The Skyrme-HF+QCM formalism presented above is applied to analyse the effect of \( T=1 \) and \( T=0 \) pairing on the binding energies of nuclei with the atomic mass \( A = N + Z \) between 20 and 100. We consider first the even-even nuclei with \( N = Z \), for which the pn pairing correlations are supposed to be the largest, and then the nuclei with \( N = Z + 2 \) and \( N = Z + 4 \).

A. Calculation scheme

To set the calculation scheme for the Skyrme-HF+QCM calculations one needs to chose the Skyrme functional, the pairing force and the model space for the pairing calculations. For the mean field we consider the Skyrme functional UNE1 [14]. The Skyrme-HF calculations have been done with the code EV8 [15], in which the mean field equations are solved in coordinate space. The mean-field is considered to have axial symmetry, so the neutron and the proton levels are double degenerate with respect to the projection of the angular momentum on the symmetry axis.
The QCM calculations are performed by solving analytically the QCM equations for the average of the pairing Hamiltonian and for the norm of the QCM wave function. This has been done by employing the Cadabra algorithm [16]. In order to keep feasible the analytical derivations, in the QCM state for the $N = Z$ nuclei (Eq. 2) we have used $n_q = 3$ while for the QCM state for $N > Z$ nuclei (Eq. 7) we have taken $n_q = 2$.

For the isovector-isoscalar pairing interaction we employ the delta force given in Eq. (11). Since the force is of zero range, the pairing calculations should be done with a finite number of single-particle states from the vicinity of Fermi levels. In the present calculations the active nucleons are allow to scatter, due to the pairing force, in 10 neutron and 10 proton single-particle states above the core defined by the QCM states (2,7).

What remains to be chosen are the strengths of the pairing forces, i.e., $V_0^{T=1}$ and $V_0^{T=0}$, or, equivalently, the strength of the isovector pairing $V_0 = V_0^{T=1}$ and the ratio $w = V_0^{T=0}/V_0^{T=1}$. How to fix these parameters is a non trivial task because there are not observables which to be related unambiguously to isovector or to isoscalar pairing. Moreover, as shown in the previous QCM calculations, the $T=1$ and $T=0$ pairing correlations always coexist and they are very difficult to disentangle because the isovector and the isoscalar counterparts of the QCM states (2,7) have a large overlap [9, 10]. The alternative we have chosen here is to perform calculations with various parameters and to keep those for which the differences between the calculated and experimental binding energies are the smallest. More precisely, we have first calculated the binding energies of a few representative even-even $N=Z$ nuclei with $V_0 = \{300, 350, 400, 465\}$ MeV/fm$^3$ and $w=0$. Then, for a given $V_0$, we have turned on the isoscalar pairing force by increasing $w$ until the value $w=2$.

B. Pairing and binding energies of $N = Z$ nuclei

The most representative results for the binding energies are presented in Fig. 1. The figure shows the binding energies residuals, i.e., the difference between the theoretical and experimental binding energies. The parameters employed in the calculations are indicated in the figure. In what follows, we shall focus on the results corresponding to the pairing force of strength $V_0=350$. First of all, it can be seen that the Skyrme-HF results, obtained by using the equal filling approximation, underestimate the binding energies by about 3-4 MeV in the middle mass region, while for the nuclei with $A > 90$ the calculated binding energies
FIG. 1: Binding energies residuals, in MeV, for even-even N=Z nuclei as a function of A=N+Z. The results correspond to the pairing forces indicated in the figure.

are larger than the experimental ones. As expected, the Skyrme-HF+BCS calculations, which take into account only the neutron-neutron (nn) and proton-proton (pp) pairing, is smoothing out the fluctuations of the HF results caused by the shell effects. For the N=Z nuclei with 60 < A < 80, where the HF fluctuations are small, in BCS approximation the residuals are decreasing by about 1 MeV compared to the HF values.

FIG. 2: Pairing energy, interaction energy and self-energy, in MeV, for 64Ge. From the left to the right are shown, for each quantity, the PBCS result and the QCM results for w=\{0.0, 1.0, 1.5, 2.0\}. pn0 and pn1 indicate the T=0 and T=1 pn channels.

From Fig. 1 it can be seen that the binding energies are increasing significantly when are taken into account the isovector pn pairing correlations, treated in the QCM approach.
On the other hand, except for $A=24$ and $A=28$, the effect of the isoscalar pn pairing on the binding energies is surprisingly small. This fact is caused by the competition between various pairing channels and between pairing and mean field. As an example, we discuss in detail the results for the nucleus $^{64}\text{Ge}$, which is illustrating a typical case.

FIG. 3: Diagonal (a) and non-diagonal (b) matrix elements of the isovector and isoscalar pairing force for $^{64}\text{Ge}$. The quantity $I_{ij}$ enumerates the pair indices of $V_{ij}$.

In Fig. 2 are shown the pairing energies for $^{64}\text{Ge}$ provided by the QCM calculations for $V_0=350$ and $w=\{0.0, 1.0, 1.5, 2\}$. In order to disentangle the pairing and the mean field effects, the results shown in Fig. 2 correspond to the calculations done on the top of the fixed mean field generated by the Skyrme-HF calculations. As a reference, in the same figure we have included also the pairing energies provided by the particle-number projected-BCS (PBCS) approach in which the variation is done after the projection. The PBCS wave function is taken as a product between a neutron and a proton pair condensate, so it does not take into account the isovector pn pairing correlations. The latter are taken into account in the isovector QCM approach ($w=0$) and, as expected, they increase the total pairing energy compared to PBCS. By contrast, the like-particle pairing energies are larger in PBCS than in QCM. This is due the fact that in isovector QCM the like-particle pairing is competing with the isovector pn pairing because they build up correlations by sharing the same model space. For the same reason, the like-particle and isovector pn pairing energies are decreasing further when the isoscalar pn channel is switched on. Yet, as seen in Fig. 2, in this case the decrease of the isovector pairing is not compensated by the pairing energy gained by
opening the isoscalar channel. On the other hand, the contribution of the isoscalar pn channel to the interaction energy is increasing rapidly with the scaling factor $w$, becoming almost equal to the isovector pn channel for $w = 1.5$. However, as seen from Fig. 2, most of the interaction energy in the isoscalar channel is coming from the self-energy. As a result, the contribution of the isoscalar pn pairing to the total pairing, in which it is not included the self-energy, is reduced significantly, much more than for the isovector pn pairing. This behavior can be traced back to the matrix elements (m.e.) of the pairing interaction, shown in Fig. 3. Thus, as seen in Fig. 3a, by increasing the scaling factor, some diagonal m.e. of the isoscalar pn pairing become larger than the isovector ones. However, the contribution of diagonal m.e. is drastically reduced when the self-energy terms are subtracted. Therefore, due to the subtraction, the dominant contribution to the pairing energies comes from the off-diagonal m.e., shown in Fig. 3b. It can be noticed that, in average, the m.e. of the isoscalar interaction are smaller than the m.e. of the isovector interaction and, more importantly, some of the isoscalar m.e. are positive. Due to these reasons, the contribution of the isoscalar pairing force to the pairing correlations is not increasing significantly with the scaling factor. In addition, in self-consistent Skyrme-HF+QCM calculations, the variation of the pairing energies can be compensated by the mean field energy. In this case, when the isoscalar channel is turned on, the mean field energy is increasing by about 530 keV for $w=1.5$ and by 540 keV for $w=2.0$, while the total pairing energy is decreasing, relative to the isovector pairing, by about the same quantity. As a consequence, as seen in Fig. 1, the total binding energy of $^{64}\text{Ge}$ is not changing much when the isoscalar pairing force is turned on.

![Graph](image1.png)

**FIG. 4:** Interaction energies (left) and pairing energies (right), in MeV, for $N = Z$ nuclei. For each nucleus are shown, from the left to the right, the results for $w = \{0.0, 1.5, 2.0\}$

The pairing energies and the interaction energies provided by the self-consistent calcula-
tions for all $N = Z$ nuclei are shown in Fig. 4. It can be seen that in the majority of nuclei these quantities have a similar pattern as in the example discussed above. In particular, we have found that when the isovector and the isoscalar interactions have the same strength ($w = 1$) the total pairing energy is smaller compared to the isovector pairing ($w = 0$) in all $N = Z$ nuclei considered in this study.

An interesting feature seen in Fig. 4 is that the pairing energies are significant for double magic nuclei $^{40}$Ca, $^{56}$Ni, for which the BCS approximation predicts no pairing. The fact that there are pairing correlations in $^{40}$Ca was also pointed out in Ref. [17]. It is worth mentioning as well that for $^{40}$Ca and $^{56}$Ni the pairing gaps extracted from the odd-even mass difference are large, of 3.6 MeV and 3.2 MeV, respectively. The gaps are also quite large, of the order of 1 MeV, in the neighboring odd-even isotopes.

FIG. 5: The residuals, function of $A = N + Z$, for $N = Z + 2$ (a) and $N = Z + 4$ (b) nuclei.

C. Pairing and binding energies of $N > Z$ nuclei

To study how the pairing correlations are affected by the extra neutrons added to $N=Z$ nuclei, we take as examples the nuclei with $N = Z + 2$ and $N = Z + 4$ and with atomic mass $20 < Z < 100$. The binding energy residuals for these nuclei are given in Fig. 5. Are shown the results for the pairing force with $V_0=350$ and $w = \{0.0, 2.0\}$. The contribution of the pairing energies to the binding energies is displayed in Fig. 6. For reference, in Fig. 6 are given also the interaction energies. The latter are increasing significantly when the
FIG. 6: Interaction energies (left) and pairing energies (right), in MeV, function of 
\(A = N + Z\), for the nuclei with \(N = Z + 2\) (top) and \(N = Z + 4\) (bottom). For each 
nucleus are shown, from the left to the right, the results for \(\omega = \{0.0, 2.0\}\)

FIG. 7: Interaction energies (left) and pairing energies (right) for \(T=0\) and \(T=1\) pn pairing 
and for \(\omega = 2.0\). The results, from the left to the right, are for the nuclei with \(N = Z\), 
\(N = Z + 2\) and \(N = Z + 4\). On x-axis is indicated the atomic mass of \(N = Z\) nuclei.

isoscalar pairing is turned on. On the contrary, this is not the case for the pairing energies. 
The reasons for that are the same as in the case of \(N = Z\) nuclei: (i) the off-diagonal m.e. 
of the interaction are less attractive for the isoscalar force; (iii) the pairing channels are 
competing with each other and also with the mean field. As a result, the binding energies of 
\(N > Z\) nuclei shown in Fig. 5 change very little when the isoscalar pairing is switched on. 
This does not mean, however, that the isoscalar pairing correlations do not contribute to the 
binding energy of \(N > Z\) nuclei. This can be seen clearly from Fig. 7, which shows how the 
pg pairing energies and interaction energies are changing by adding neutrons to the \(N = Z\)
nuclei. In both T=0 and T=1 channels these energies are decreasing when more neutrons are added. However, they are not vanishing, including for the nuclei with $N = Z + 4$, and they coexist in all the nuclei. In fact, this is happening not only for the large isoscalar strength considered here, but also for any QCM calculations with an isovector-isoscalar pairing force with $w > 0$.

IV. SUMMARY AND CONCLUSIONS

We have discussed the contribution of isovector and isoscalar pairing on binding energies of $N = Z$ nuclei and of $N > Z$ nuclei with $N = Z + 2$ and $N = Z + 4$. The binding energies have been obtained by performing self-consistent Skyrme-HF+QCM calculations in the intrinsic system. An interesting aspect pointed out by these calculations is the strong interdependence between all types of pairing correlations. In particular, when the isoscalar pn pairing channel is switched on, the pairing correlations are redistributed among all the pairing channels without changing significantly the total pairing energy. Due to this reason, for the majority of $N \approx Z$ nuclei the binding energy is not affected much when the isoscalar pairing channel is switched on. Yet, in all the calculations which include both the isovector and the isoscalar pairing forces, the isoscalar pairing correlations contribute significantly to the binding energies and coexist always with the isovector pn pairing. This feature, discussed already in the previous studies [9, 10], is related to the exact conservation of the particle number and the isospin by the QCM approach.

The present Skyrme-HF+QCM calculations are based on two approximations which should be further checked and improved. Thus, on one hand, since the calculations are done in the intrinsic system, the ground states have not a well-defined angular momentum. On the other hand, in the isoscalar pairing channel are considered only proton-neutron pairs in time-reversed states. This is a rather common choice when the pairing calculations are done with a deformed mean field [18]. In principle, should be also introduced the correlations corresponding to proton-neutron pairs with $S = 1, S_z = \pm 1$. How to treat these correlations in self-consistent Skyrme-HF+QCM calculations is a non-trivial task which will be addressed in a future study.
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