A quartet BCS-like theory

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Abstract

We introduce a BCS-like theory for the quartet correlations induced by the isovector pairing interaction. It is based on a coherent state of BCS type and, unlike usual mean field approaches, it displays a vanishing pair anomalous density \( \langle c^\dagger c^\dagger c c \rangle = 0 \). We find good agreement between our theory and the exact results. We discuss how the pairing and quarteting correlations share some similar qualitative features within the BCS approach. However, there is no sharp quarteting phase transition. We also present various ways in which our theory may be further developed.

Keywords:
Quartet correlations, proton-neutron pairing

Introduction

The advances in the experimental techniques of the last three decades have opened up new possibilities to investigate the nature of the nuclear interactions at the \( N = Z \) line. The significant overlap between neutron and proton orbitals in this region allows the existence of proton-neutron \( \langle pn \rangle \) pairing, which is suppressed away from \( N = Z \).

Already in the first theoretical approach to \( pn \) pairing dating six decades ago, Belyaev, Zacharev and Soloviev realized that “one must take into consideration the quadruple correlation of particle-like nucleons in addition to pair correlations” \[1\]. Subsequent works proposed various ways to incorporate these quartet correlations into a functioning theory, e.g. those of Flowers and Vujčić \[2\] and of Brémont and Valatin \[3\]. More recently, Civitarese, Reboiro and Vogel \[4\] concluded that “an isospin-symmetric Hamiltonian, treated with the generalized Bogolyubov transformation, fails to describe the ground state properties correctly”. This transformation naturally diagonalizes the Hamiltonian in the mean field approximation, i.e. upon the replacement of some operators associated with large matrix elements by their expectation value. In our case, the monopole pair operators \( P^\dagger \) are replaced by the pairing anomalous density \( P^\dagger \rightarrow \langle P^\dagger \rangle \). The existence of only pair condensates in the case of \( pn \) pairing should thus be carefully considered.

Nevertheless, the standard mean field approach to pairing in \( N = Z \) nuclei has been for many years the generalized Hartree-Fock-Bogoliubov approximation \[5\], where all types of Cooper pairs are treated in a unified manner. In the last decade, the particle number and isospin conserving Quartet Condensation Model (QCM) was proposed for the study of isovector pairing and quarteting correlations in \( N = Z \) nuclei \[6, 7\]. It was further developed in Refs. \[8, 9, 10, 11, 12, 13\] to the case of isoscalar pairing and \( N > Z \) nuclei. General microscopic quartet models for a shell-model basis with an effective Hamiltonian were also recently proposed \[14, 15, 16, 17, 18, 19\]. In these approaches, the basic building blocks are not the Cooper pairs anymore, but four-body structures composed of two neutrons and two protons coupled to the isospin \( T = 0 \) and to the angular momentum \( J = 0 \), denoted “\( \alpha \)-like quartets”. Interesting connections between the symmetry restricted pair condensate and the quartet descriptions have very recently been uncovered \[20\]. However, as to this day, “no symmetry-unrestricted mean-field calculations of \( pn \) pairing, based on realistic effective interaction and the isospin conserving formalism have been carried out” \[20, 21\].

In this work, we take a step along this direction. We construct a solvable BCS-like theory of quartet correlations without assuming any mean field approximation, but only a coherent state ansatz of BCS type involving the isoscalar quartet operator. At variance with the quartet BCS theory of Schuck et al \[22\], solving our simpler model requires no approximation.

Formalism

The system of interest consists of a number \( N = Z \) of neutrons and protons moving outside a self-conjugate inert core, and interacting through a charge-independent pairing force. The isovector pairing Hamiltonian is suitable to describe both spherical and deformed nuclei,

\[
H = \sum_{i=1}^{N_N} \epsilon_i N_{i,0} + \sum_{\tau=0,\pm1} \sum_{j=1}^{N_N} V_{ij} P_{ij}^\dagger P_{ij},
\]

where \( i, j \) denote the single particle doubly-degenerate states and \( \epsilon_i \) refers to the single particle energies; a time conjugated state will be denoted by \( \bar{i} \). The \( N_{i,0} \) operator counts the total number of particles, \( N_{i,0} = N_{i,1} + N_{i,-1} = \sum_{\nu=\pm1} (c_{i,\nu}^\dagger c_{i,\nu}^\dagger + c_{i,\nu}^\dagger c_{i,\nu}) \), and the isovector triplet of pair operators is given by \( P_{i,1}^\dagger = c_{i,0}^\dagger c_{i,1}^\dagger P_{i,-1} = c_{i,1}^\dagger c_{i,-1}^\dagger P_{i,0} = \)
\[ Q^j(x) \equiv \prod_{i=1}^{N_{\text{ev}}} x_i P^j_{i,1} \], which depend on a set of mixing amplitudes \( x_i, i = 1, 2, \ldots, N_{\text{ev}} \). A collective quartet ansatz is then constructed by coupling two collective pairs to the total isospin \( T = 0 \),

\[ Q^j(x) \equiv \prod_{i=1}^{N_{\text{ev}}} x_i P^j_{i,1} - \prod_{i=1}^{N_{\text{ev}}} (x_i)^2 . \] (2)

For \( N = Z \) nuclei, the ground state of the Hamiltonian (1) is taken to be a "condensate" of such \( a \)-like quartets, \( \Psi(x) = |Q(x)\rangle \rho(0) \), where \( n_q \) is the number of quartets. The concept of a "condensate" denotes here the state obtained by acting with the same operator a number of times on the vacuum. It should not be confused with an ideal boson-type condensate. The model is solved by determining numerically the mixing amplitudes \( x_i \) upon the minimization of the Hamiltonian expectation value subject to the unit norm constraint, i.e., \( \delta(\Psi(x)H\Psi(x)) = 0, \langle \Psi(x)\Psi(x) \rangle = 1 \).

The quartet state has, by construction, a well defined particle number and isospin. As such, it may be well suited to precisely determine within the QCM. The formulation of this model is based on correlated four-particle structures known as "quartets". To obtain a quartet, one first defines a set of collective \( \pi\pi, \nu\nu \) and \( \pi\nu \) Cooper pairs \( \Gamma_i^j(x) \equiv \sum_{j=1}^{3} x_j P^j_{i,j} \), which is considerably more complicated. To see this, consider the Brémond-Valatin factorized ansatz (which by itself misses most of the relevant correlations). As such, the QBCS state is a superposition of all possible factorized states, each having the relative amplitude of finding a pair on the level \( i \) proportional to \( x_i \) and that of finding a quartet to \( x_i^2 \). Note that, while the factorized Brémond-Valatin may be treated by a quasi-particle transformation, the integration necessary to obtain the QBCS state completely destroys the quasi-particle picture.

As a first step, in the present work we limit ourselves to assessing the consequences of breaking only the particle number conservation; we leave the breaking of isospin conservation to future investigations. We compute the ground state correlations within the QBCS model by minimizing the expectation value of \( E(x) = \langle QBCS| H - \lambda N_0 |QBCS\rangle / \langle QBCS|QBCS\rangle \) subject to the particle number constraint \( \langle QBCS|N_0|QBCS\rangle / \langle QBCS|QBCS\rangle = 4n_q \), where \( n_q \) is the number of quartets, \( n_q = (N + Z)/4 \). The expressions of the norm of and of the various operator averages on the QBCS state as functions of the mixing amplitudes may easily be extracted from Eq. (6). Here, for illustrative purposes we just compare the QBCS and BCS norm functions in the simplest case of \( N_{\text{ev}} = 2 \); for the QBCS we obtain \( \langle QBCS|QBCS\rangle = |QBCS|QBCS\rangle = |QBCS| \sqrt{2} = \langle QBCS|QBCS\rangle = 4n_q \).
225x_1^4 x_2^4 + 12x_1^3 x_2^2 + 9x_1^2 x_2 + 9x_1 x_2^2 + 1, while the BCS norm is just 
\langle BCS|BCS \rangle = x_1^2 x_2^2 + x_1^2 + x_2^2 + 1. While the BCS norm may be 
factorized as 
\langle BCS|BCS \rangle = (1 + x_1^2)(1 + x_2^2), the QBCS norm 
does not admit any factorization.

A similar behaviour is valid for the other relevant quantities 
of the theory, which are given by more complicated expression 
in the QBCS case than in the standard BCS (see the general 
expressions given in the Supplementary Material).

Let us finally remark that the QBCS ground state of Eq. (3) 
contains only components where the particle number is a mul-
tiple of 4. Hence, there is no pair anomalous density in our 
theory, i.e. \langle QBCS|P_{ij} QBCS \rangle = 0. There is, however, a four-
body anomalous density, which we analyze below.

Numerical results. We test our formalism against the well 
established QCM in the nuclei above 100Sn and above 16O. We consider the same model spaces and interactions as in 
Refs. 6, 8, namely the spherical spectrum \epsilon_{2d_{5/2}} = 0.0MeV, 
\epsilon_{1g_{7/2}} = 0.2MeV, \epsilon_{2d_{3/2}} = 1.5MeV, \epsilon_{3p_{3/2}} = 2.8MeV together 
with the effective Bonn A potential of Ref. 23 for the sdg shell 
and the spectrum \epsilon_{1d_{3/2}} = -3.926MeV, \epsilon_{2s_{1/2}} = -3.208MeV.
\[ \epsilon_{\text{sd}} = 2.112 \text{MeV} \] together with the USDB interaction of Ref. [24] for the \textit{sd} shell. We solve the QCM model using the analytical method of Refs. [25, 26].

We show in Fig. (1) the results for the correlations energies defined as \( E_c = E_0 - E \), where \( E \) is the energy of the ground state and \( E_0 \) is the energy calculated without taking into account the isovector pairing interaction. In both cases, we observe good agreement between the QBCS and the particle number conserving QCM, with relative errors of at most 6% for the \(^{16}\text{O}\) core and 10% for the \(^{100}\text{Sn}\) core (note that, at variance with the particle number projected BCS, the QCM offers practically the exact solution, within 1% error). A very good agreement is obtained also for the average level occupancies, shown in Fig. (2) for the nuclei at shell half-filling.

As mentioned above, there is no anomalous pair density in the QBCS theory, \( \langle P \rangle = 0 \). As an indicator of the four body correlations, we choose to study the quartet anomalous density defined in analogy to the quantity appearing in the standard pairing case, \( \langle BCS|\mathcal{F}_1(x_i = 1)|BCS \rangle \), related to the pairing gap. Similarly to the standard pairing case, the quartet anomalous density exhibits minima at the open and closed shell configurations and a maximum around shell half-filling, as seen from Fig. (4).

Thus far, the pairing and quarteting correlation treated within the BCS and, respectively, QBCS formalisms appear to show quite similar manifestations. The main difference arises when considering the response of the quartet correlations to a varying interaction strength. It is well known that the standard BCS has a nontrivial solution only for interaction strengths greater than a critical value dependent on the model space.

In the QBCS case we observe no evidence of a sharp transition from a quarteting to a normal phase as we decrease the interaction strength. As seen from Fig. (5) when scaling the interaction matrix elements by a factor \( \kappa \in [0, 1] \) the correlation energy and its derivative versus the interaction strength scaling factor \( \kappa \), for the nuclei \(^{28}\text{Si}\) and \(^{120}\text{Nd}\).
energy varies smoothly, with no jumps of its derivative. Instead, there is a relatively narrow interval towards small values of the scaling factor $\kappa$ where the derivative experiences a more pronounced variation. This behaviour of the QBCS (which does not conserve the particle number) is exhibited also by the number projected BCS theory. We conclude that the restoration of the isospin symmetry is enough to smoothen the transition from the quarteting to the normal phase.

**Conclusions.** We proposed a BCS-like theory for quartet correlations based on a quartet coherent state analogous to the famous $|BCS\rangle$ state. Our ansatz is unique as it does not contain any pairing anomalous density $\langle P \rangle$ (as opposed to usual mean field treatments for $pn$ pairing), but instead one of quartet type $\langle Q \rangle$. We evidenced that the standard pairing and quarteting correlations share similar qualitative features, but there is no sharp quarteting transition. Additionally, we uncovered new connections between the quartet models and some of the early BCS-like attempts to $pn$ pairing.

The QBCS theory is flexible and there are numerous ways in which it may be expanded. On the one hand, extra neutron pairs may be included for the study of $N > Z$ nuclei by considering an ansatz of the form $|QBCS(N > Z)\rangle = \exp(\Gamma^+(y))\exp(Q^+(y))|0\rangle$, containing both neutron pairs and quartets as building blocks. On the other hand, combined isovector and isoscalar interactions may be treated with the ansatz $|QBCS(iv + is)\rangle = \exp(\hat{Q}_{iv}^+(x) + \hat{Q}_{is}^+(y))|0\rangle$.

The excited states of the QBCS model may be computed by minimizing the energy function subject to the additional constraint of zero overlap with the ground state. Although a quasiparticle picture would be preferred, recent results also indicate that it may be inappropriate for quartet correlations. Nevertheless, an approximate quasiparticle description may be obtained within a boson formalism along the lines of Ref. [28]. Note that, in deriving the expressions for the averages of the various operators on the QBCS states starting from Eq. (6), one may as well treat the pair operators $p_j$, as bosons and still obtain the exact fermionic results.

Lastly, let us remark that the coherent quartet ansatz of Eq. (2) is still rather restrictive. More generally, one should consider the case of non-separable mixing coefficients, i.e. $Q_j = \sum_{i \neq j} X_{ij} (2p_i \cdot P_j^\dagger - P_i \cdot P_j^\dagger )$ with $X_{ij} \neq x_ix_j$. This more complex case may also be treated by taking advantage of the properties of Gaussian integration. In this case we obtain

$$|QBCS\rangle = \exp(Q^+)|0\rangle = \exp(\sum_{ij} \beta_{ij} X_{ij} P_j^\dagger)|0\rangle =$$

$$= \int d^{3N_{nu}} Z \exp \left[ - \sum_{ij} Z_{ij} (x^{-1})_{ij} z_{ij} \right] \times \prod_{j=1}^{N_u} (1 + z_j \cdot P_j^\dagger + z_j^2 Q_j^+ / 2)|0\rangle ,$$

where a scalar product is understood in all expressions involving two vectors. The norm and the averages of the various operators on the QBCS state may be automatically computed as Wick contractions of various $X_{ij}$’s by using the Wick theorem for multidimensional Gaussian integrals [29].

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**References**

[1] B. N. Belyaev, V. B. Zacharev, V. G. Solovev, Superfluidity of light nuclei, J. Exptl. Theoret. Phys. 38 (1960) 952.

[2] B. Flowers, M. Vujii, Charge-independent pairing correlations Nuclear Physics 49 (1963) 586–604. doi:10.1016/0029-5582(63)90123-8 URL http://www.sciencedirect.com/science/article/pii/0029558263901238

[3] B. Brumond, J. Valatay, A method to describe pairing correlations of protons and neutrons Nuclear Physics 41 (1964) 640–659. doi:10.1016/0029-5582(63)90543-1 URL http://www.sciencedirect.com/science/article/pii/0029558263905431

[4] O. Civitarese, M. Reboiro, P. Vogel, Neutron-proton pairing in the boson approach Phys. Rev. C 56 (1997) 1840–1843. doi:10.1103/PhysRevC.56.1840 URL https://link.aps.org/doi/10.1103/PhysRevC.56.1840

[5] A. L. Goodman, Proton-neutron pairing in $Z = N$ nuclei with $A = 76 – 96$, Phys. Rev. C 60 (1999) 014311. doi:10.1103/PhysRevC.60.014311 URL https://link.aps.org/doi/10.1103/PhysRevC.60.014311

[6] N. Sandulescu, D. Negrea, J. Dukelsky, C. W. Johnson, Quartet condensation and isovector pairing correlations in $N = Z$ nuclei Phys. Rev. C 85 (2012) 061303. doi:10.1103/PhysRevC.85.061303 URL https://link.aps.org/doi/10.1103/PhysRevC.85.061303

[7] D. Negrea, Proton-neutron correlations in atomic nuclei Ph.D. thesis, University of Bucharest and University Paris-Sud (2013). URL https://tel.archives-ouvertes.fr/tel-00870588/document

[8] N. Sandulescu, D. Negrea, C. W. Johnson, Four-nucleon $\alpha$-type correlations and proton-neutron pairing away from the $N = Z$ line Phys. Rev. C 86 (2012) 041302. doi:10.1103/PhysRevC.86.041302 URL https://link.aps.org/doi/10.1103/PhysRevC.86.041302

[9] D. Negrea, N. Sandulescu, Isovector-proton-neutron pairing and Wigner energy in Halo Nuclei Phys. Rev. C 90 (2014) 024322. doi:10.1103/PhysRevC.90.024322 URL https://link.aps.org/doi/10.1103/PhysRevC.90.024322

[10] N. Sandulescu, D. Negrea, J. Dukelsky, C. W. Johnson, Proton-neutron pairing and alpha-type quartet condensation in nuclei Journal of Physics: Conference Series 533 (2014) 012018. doi:10.1088/1742-6596/533/1/012018 URL https://doi.org/10.1088/1742-6596/533/1/012018

[11] N. Sandulescu, D. Negrea, D. Gambacurta, Proton-neutron pairing in $N=Z$ nuclei: Quartetting versus pair condensation Physics Letters B 751 (2015) 348–351. doi:10.1016/j.physletb.2015.10.063 URL http://www.sciencedirect.com/science/article/pii/S0370269315308067

[12] D. Negrea, N. Sandulescu, D. Gambacurta, Isovector and isoscalar pairing in oddodd $N Z$ nuclei within a quartet approach Progress of Theoretical and Experimental Physics 2017 (7), 073D05 (7 2017). arXiv: http://oup.prod.sis.lan/ptep/article-pdf/2017/7/073D05/19371736.pdf; doi:10.1093/ptep/ptx071 URL https://doi.org/10.1093/ptep/ptx071

[13] D. Negrea, P. Buganu, D. Gambacurta, N. Sandulescu, Isovector and isoscalar proton-neutron pairing in $N > Z$ nuclei Phys. Rev. C 98 (2018) 064319. doi:10.1103/PhysRevC.98.064319 URL https://link.aps.org/doi/10.1103/PhysRevC.98.064319

[14] J. Feng, Y. Lei, Y. M. Zhao, S. Pineda, A. Anima, Nucleon-pair approximation of the shell model with isospin symmetry
We present here some computational details regarding the general expressions of the norm and various operator averages occurring in the QBCS theory.

The norm of the QBCS state may be written as a double integral

\[ \langle QBCS | QBCS \rangle = \frac{1}{(4\pi)^3} \int d^3w d^3\zeta \exp\left(-\frac{\zeta^2}{4} - \frac{w^2}{4}\right) \times \prod_{i=1}^{N_{lev}} \left[ 0 \right] + x_i \zeta \cdot \mathbf{p}_i + x_i^2 \zeta^2 q_j^+ \left[ 0 \right] / 2 \right] / 2 \right] / 2 \right] / 2 \] \]

The integration may be trivialized by passing to spherical coordinates,

\[ \langle QBCS | QBCS \rangle = \frac{1}{8\pi} \int_0^\infty dw \, w^2 \exp\left(-w^2/4\right) \int_0^\infty dz \, z^2 \exp\left(-z^2/4\right) \times \prod_{i=1}^{N_{lev}} \left( 1 + x_i \zeta \cdot \mathbf{z} + x_i^2 \zeta^2 / 4 \right) . \]

Using some well-known properties of Gaussian integration, this expression (and those presented below) may be easily evaluated for any number of levels. The single particle term reads

\[ \langle QBCS | QBCS \rangle = \frac{1}{(4\pi)^3} \int d^3w d^3\zeta \exp\left(-\frac{\zeta^2}{4} - \frac{w^2}{4}\right) \times \prod_{i=1}^{N_{lev}} \left( 1 + x_i \zeta \cdot \mathbf{z} + x_i^2 \zeta^2 / 4 \right) . \]

The interaction term is decomposed into diagonal and nondiagonal parts,
The diagonal part is

\[
\langle \text{QBCS} | \sum_k V_{kk} \sum_{\alpha=1}^3 p^{\dagger}_{k,\alpha} p_{k,\alpha} | \text{QBCS} \rangle = \frac{1}{(4\pi)^2} \int d^3 wd^3 z \exp \left( -\frac{z^2}{4} - \frac{\bar{w}^2}{4} \right) \times \\
\sum_{k=1}^{N_{\text{loc}}} 3V_{kk}(x_k^2 \bar{w} \cdot \bar{z} + x_k^4 \bar{w}^2 \bar{z}^2 / 4) \prod_{i \neq k} (1 + x_i^2 \bar{w} \cdot \bar{z} + x_i^4 \bar{w}^2 \bar{z}^2 / 4)
\]

(15)

The non-diagonal part is

\[
\langle \text{QBCS} | \sum_{k \neq l} V_{kl} \sum_{\alpha=1}^3 p^{\dagger}_{k,\alpha} p_{l,\alpha} | \text{QBCS} \rangle
\]

\[
= \frac{1}{(4\pi)^2} \int d^3 wd^3 z \exp \left( -\frac{z^2}{4} - \frac{\bar{w}^2}{4} \right) \times \\
\sum_{k \neq l} V_{kl}(x_k x_l (1 + x_k^2 x_l^2 \bar{w}^2 \bar{z}^2 / 4) \bar{w} \cdot \bar{z} + x_k x_l (x_k^2 + x_l^2) \bar{z}^2 \bar{w}^2 / 2) \times \\
\prod_{i \neq k, l} (1 + x_i^2 \bar{w} \cdot \bar{z} + x_i^4 \bar{w}^2 \bar{z}^2 / 4)
\]

(16)

Similar expressions may be easily obtained for the quartet anomalous density and for the square of the total particle number operator.