How to count nucleon pairs?

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Abstract

Within the context of the isovector-pairing SO(5) model, three methods measuring numbers of different kinds of nucleon pairs are discussed. Though methods do not give the same results, the odd-even staggering in pair numbers in even-even and odd-odd $N = Z$ nuclei and the reduction of the np-pair number with increasing $T_z$ is observed in all three procedures.

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Structures comprised of nucleon pairs are influential in describing nuclear states. The most important pairing degree of freedom is the monopole pair with $L = 0$ orbital angular momentum. In medium-heavy and heavy nuclei, the monopole pairing pertains to pairs of like nucleons as valence protons and neutrons occupy different shells and cannot couple to $L = 0$. Today, considerable experimental activity is aimed at study of proton-rich nuclei. In those, the neutron-proton-pairing mode becomes notable.

In a recent paper [1], a method has been suggested to quantify effects of different pairing modes and measure pair numbers in the nuclear-wave function. We should emphasize that the pair numbers are not directly observable quantities. Even in simple models of pairing, there is no operator that counts nucleon pairs. If an exact solution of the problem is available, one need not to operate with the pair numbers. Their quantification can, however, make the problem more transparent. Also in complex situation, the notion of the significance of different pairs may be helpful in constructing approximate solutions and/or devising model descriptions.

In the present study, we examine the measure of pair numbers of Ref. [1] and suggest alternative procedures. As in Ref. [1], we discuss the problem within the context of a simple model of monopole-isovector pairing with the

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underlying O(5) algebraic structure \cite{2}. The model reflects pairing features of realistic shell-model calculations \cite{3}.

In the monopole-isovector-pairing model, the set of pair creation operators

\[ S^\dagger_\nu = \frac{1}{\sqrt{2}} \sum_j [a_j^{\dagger \frac{1}{2}} a_j^{\frac{1}{2}}]_{0\nu} , \tag{1} \]

the conjugate pair annihilation operators \( S_\nu \), the isospin operator \( T \), and the total number operator \( \hat{N} \) closes the O(5) algebra. The degeneracy of the shell is \( 4\Omega = 2 \sum (2j + 1) \). The problem of the SO(5) pairing Hamiltonian

\[ H = -G \sum_\nu S^\dagger_\nu S_\nu , \tag{2} \]

can be solved algebraically. We shall consider the seniority zero eigenstates \( |N TT_z\rangle \) of \( H \) labelled by half the number of nucleons \( N \), isospin \( T \), and isospin \( z \)-projection \( T_z \).

The basic building blocks of the SO(5) model space are the nn-, pp-, and np-pair creation operators. We shall examine possible procedures which would estimate the average numbers \( \langle N_{nn} \rangle \), \( \langle N_{pp} \rangle \), and \( \langle N_{np} \rangle \) of the respective pairs in a given state.

Within the O(5) algebra, there are no operators which could be considered as the number operators of particular pairs. There are, however, two operators which relate the different pair numbers. Namely, the sum of the pair numbers should give half the number of nucleons

\[ \langle N_{nn} \rangle + \langle N_{pp} \rangle + \langle N_{np} \rangle = N \tag{3} \]

and the difference between nn- and pp-pair numbers should link with the charge of the state

\[ \langle N_{nn} \rangle - \langle N_{pp} \rangle = T_z . \tag{4} \]

In Ref. \cite{4}, the operator

\[ N_{nn}^\dagger = \frac{1}{\Omega} S_1^{\dagger} S_1 \tag{5} \]

and the analogously defined operators \( N_{pp}^\dagger \) and \( N_{nn}^\dagger \) have been suggested as measures of the numbers of different pairs. We denote this method by I. In this method, the pair numbers are associated with the contributions of the respective pairing terms in the Hamiltonian (2) to the total energy and the relations can be obtained

\[ \langle N_{nn}^\dagger \rangle + \langle N_{pp}^\dagger \rangle + \langle N_{np}^\dagger \rangle = N \left(1 - \frac{N - 3}{2\Omega} \right) - \frac{1}{2\Omega} T(T + 1) \tag{6} \]
\[ \langle N_{nn}^{I} \rangle - \langle N_{pp}^{I} \rangle = T_z (1 - \frac{N - 1}{\Omega}) \]  

\[ \langle N_{np}^{I} \rangle = \frac{1}{3} N (1 - \frac{N - 3}{2\Omega}) - \frac{1}{6\Omega} T(T+1) \]
\[ - \frac{1}{3} \frac{3T_z^2 - T(T+1)}{(2T-1)(2T+3)} [(1 - \frac{N - 1}{\Omega})(2N+3) \]
\[ + \frac{1}{\Omega} (N + T + 1)(N - T) \] .

For the large shell degeneracy \( \Omega \) or more strictly speaking for \( N \ll \Omega \), the pair operators exhibit boson-like behaviour and the pair numbers in method I obey Eqs. (3) and (4). For nuclei around the middle of the shell, however, serious discrepancy between (3) and (7) and the natural constraints (3) and (4) on pair numbers may occur. One can remedy the total pair number condition by scaling simply pair numbers in method I (and we shall use this procedure in the following). Anyhow, the charge constraint (4) will not be fulfilled.

This deficiency puts some question on the method I as a measure of different pair numbers. Certainly, operators (3) quantify contributions of different pairing terms in Hamiltonian (2). In many-pair states, however, those are influenced by the Pauli principle and the relation to the pair numbers is not immediate and even may be misleading.

We shall propose an alternative method II for obtaining the pair numbers that employs directly the pair basis. In that the states are constructed as

\[ |N_{nn} N_{pp} N_{np} \rangle = a S_1^{S_{nn}} S_{-1}^{S_{pp}} S_0^{S_{np}} |0\rangle , \]

where \( a \) normalizes the state (9). The use of the pair basis in calculating the average pair numbers is not straightforward. Namely, the pair basis is not orthogonal and for \( N > \Omega \) is even overcomplete. Nevertheless, the squared overlap of the pair state (9) with a wave function \(|\psi\rangle\) gives certainly a probability of the occurrence of the state with given pair numbers. We are thus tempted to define the average pair numbers as

\[ \langle N_{nn}^{II} \rangle = C \sum N_{nn} \langle N_{nn} N_{pp} N_{np} | \psi \rangle^2 \]

with the scaling factor

\[ C = \sum \langle N_{nn} N_{pp} N_{np} | \psi \rangle^2 \]

and similarly for \( \langle N_{pp}^{II} \rangle \) and \( \langle N_{np}^{II} \rangle \). Note that \( C \) scales the definition (10) so that Eqs. (3) and (4) are obeyed. In the limit of large \( \Omega \), pair numbers from method II agree with those from method I.
The complications in the preceding two definitions (5) and (10) of pair numbers are connected with the fact that we intend to implement the boson-like behaviour to pair operators that do not obey the boson commutation relations exactly unless \( \Omega \) is large. This mirrors in the insufficiency of the method I to fulfill the charge constraint (4) and in the necessity to deal with the nonorthogonal basis in the method II.

There exists a possibility to rephrase the fermion problem in the boson language. For the bifermion O(5) algebra, the Dyson boson realization has been constructed in Ref. [5]. In our specific isovector-pairing case, the boson space is formed from the scalar-isovector boson \( s_{\nu} \). The fermion-pair operators are mapped on the boson operators as

\[
S_{\nu}^\dagger \rightarrow (\Omega - \frac{1}{2} \hat{N} + 1)s_{\nu}^\dagger + (-)^{\nu}\frac{1}{2} s_{\nu}^\dagger \cdot s_{-\nu}^\dagger , \\
S_{\nu} \rightarrow s_{\nu} .
\]

Using the above relations, the boson image \( H_B \) of the Hamiltonian \( H \) is constructed. When \( H_B \) is diagonalized in the ideal (Fock) boson space, all the eigenvalues and boson images of eigenstates of the original fermion problem are provided. The dimension of the ideal boson space can be larger that that of the fermion task. For the SO(5) Hamiltonian, spurious states occur in the boson picture for \( N > \Omega \). They, however, clearly separate from the physical solutions for example by the isospin value.

We may make use of the boson formulation of the fermion problem to get the boson-like fermion-pair numbers. The bosons are images of the fermion pairs. In the boson space, the boson number operators \( \hat{n} \) are well defined. We identify the average boson numbers with another measure (method III) of the pair numbers

\[
\langle N_{III}^{nn} \rangle = \langle \hat{n}_{s_1} \rangle
\]

and similarly for \( \langle N_{III}^{pp} \rangle \) and \( \langle N_{III}^{np} \rangle \). Here, the boson eigenvectors are denoted by the round brackets. Such a definition of pair numbers obeys Eqs. (3) and (4). Explicitly, one gets

\[
\langle N_{III}^{np} \rangle = \frac{1}{3} N - \frac{1}{3} \frac{3T^2 - T(T + 1)}{2T - 1)(2T + 3)} (2N + 3) .
\]
Fig. 1. The pair numbers for the SO(5) model ground state in \( N = Z \) nuclei. The filled circles, triangles, and hollow circles refer to methods I, II, and III, respectively. Alternatively, the boson definition (12) of pair numbers is obtained from the method I employing the pairing force when the \( 1/\Omega \) corrections are neglected. One cannot, however, deduce that the definition (12) is inferior to that of (5). The \( 1/\Omega \) corrections reflect the Pauli principle and deviations of the pair behaviour from the boson one. On the other hand, we would like to understand the pair numbers which are the boson-like quantities. Simple relations of Eqs. (3) and (4) for the pair numbers should hold which are in the method I deteriorated just by the \( 1/\Omega \) terms.

As it is seen from Fig. 1, all three methods give very similar quantities for the average pair numbers in the ground states of \( N = Z \ f p \) shell nuclei. The odd-even staggering observed in Ref. [1] is thus confirmed also by another two measures of the numbers of different pairs.

In Fig. 2 on the left, the pair numbers for even-even Fe isotopes are shown. Here, the three methods differ more pronouncedly than for the case of Fig.

\footnote{In the present SO(5) case, we know the results in method I analytically and can perform the \( \Omega \to \infty \) limit without resorting to the boson formulation. In the general case, the diagonalization in the boson space is necessary.}

\footnote{Note that the proximity of the results of the methods I and III does not mean that the \( 1/\Omega \) corrections in (5) are small. We remind that the pair numbers from the definition (5) are scaled to sum to the total number of pairs.}
Fig. 2. The pair numbers for the SO(5) model ground state in even-even Fe and odd-odd Co nuclei. The filled circles, triangles, and hollow circles refer to methods I, II, and III, respectively. The full lines connect \( \langle N_{\text{nn}} \rangle \) points, the dash-dotted lines connect \( \langle N_{\text{pp}} \rangle \) points, and the dashed lines connect \( \langle N_{\text{np}} \rangle \) points.

Nevertheless, the alternative methods confirm a decrease of the number of np pairs with increasing \( T_z \) noticed in Ref. [1]. In the method I, numbers of nn and pp pairs increase with increasing \( T_z \) and significantly break down the charge condition (4). On the other hand, in methods II and III that fulfil the charge constraint, a rough constancy of the number of pp pairs and linear increase of the number of nn pairs is observed when the neutrons are added to the nucleus. In Fig. 2 on the right, the odd-odd Co isotopes exhibit a similar behaviour with increased importance of the np pair as compared to even-even case.

When \( T_z \) is increasing, the decrease of the number of np pairs suggests a diminishing role of the np pairing. It would be important to be able to judge at what value of \( (N - Z) \) one can neglect the np-pairing degree of freedom and approximate the ground state as a product of nn and pp paired states. The exactly solvable SO(5) model makes possible such a discussion. The exact ground-state wave function of the Hamiltonian (2) for the even-even nucleus is written up to the normalization factor as

\[
|\mathcal{N} T = T_z T_z \rangle \sim (S^\dagger \cdot S^\dagger)^{(N - T_z)/2} S_i^{(T_z)} |0\rangle
\]  

(14)

whereas for the odd-odd nucleus we have

\[
|\mathcal{N} T = T_z + 1 T_z \rangle \sim (S^\dagger \cdot S^\dagger)^{(N - T_z - 1)/2} S_i^{(T_z)} S_0 |0\rangle.
\]  

(15)

The important building block of the ground-state wave function is the two-pair
The exact ground-state energy (in units of $G$) (hollow circles) and the mean value of $H$ in the approximate state with no np correlations (filled circles) are given. In the lower part, the squared overlap of the exact and approximate wave functions is shown.

$T = 0$ structure

$$S_0^\dagger S_0^\dagger - 2S_1^\dagger S_{-1}^\dagger .$$

From that the $T = 0$ even-even core is constructed to which an appropriate number of nn pairs and one np pair for the odd-odd case is added.

We shall approximate the SO(5) ground state by discarding the np part in the above two-pair $T = 0$ structure (16). The isospin is then mixed in the approximate solution. For the even-even nucleus, we have

$$|NT_z, \text{no np correlations}\rangle \sim S_1^{\dagger (N+T_z)/2} S_{-1}^{\dagger (N-T_z)/2} |0\rangle .$$

Of course, at least one np pair must be present for the odd-odd nucleus

$$|NT_z, \text{no np correlations}\rangle \sim S_1^{\dagger (N+T_z-1)/2} S_{-1}^{\dagger (N-T_z-1)/2} S_0^\dagger |0\rangle .$$

In the upper part of Fig.3, the exact ground-state energy is compared with the mean value of $H$ in the approximate state with no np correlations. In the lower part of Fig.3, the squared overlap of the exact and approximate wave functions is shown. Fig.3 corresponds to the findings inferred from the analysis of pair numbers. The diminishing role of the np pair with increasing $T_z$ is particularly exhibited in the even-even case. In the odd-odd nucleus, the mandatory np pair stabilizes the np-pairing degree of freedom and there is
a little overlap between the exact state and the wave function with the np
correlations neglected for small values of $T_z$. Here, however, the increase of
the overlap is more abrupt than in the even-even case. For $(N - Z) = 10$ both
in the even-even and odd-odd case, the exact wave function overlaps with the
wave function with no np correlations by more than 90%.

Note also that the exact and approximate ground-state energies might not
differ much even if the overlap is small. The leading term in the ground-state
energy is given as $-G\Omega N$ irrespective of the actual form of the wave function.
The binding energies alone are not thus best quantities to judge about the
np correlations and about the quality of an approximate wave function. One
should resort to difference filters, such as that of Ref. [4], in which the leading
term contribution is eliminated.

If the isospin symmetry is violated in the SO(5) Hamiltonian and the np-
pairing force is set to zero, one would expect that the number of np pairs
should go to zero. However, the methods I and II give a nonzero average
number of np pairs in this case. Similarly, in the O(8) space including the
isoscalar pair [5], the number of isoscalar pairs is nonzero for the Hamiltonian
with the isoscalar pairing switched off in methods analogous to (4) and (10).
On the other hand, the boson method III of counting pairs gives a null number
for the pairing mode whose pairing term is not present in the Hamiltonian.

To conclude, we stress again that counting the number of pairs in a fermion
state is not well and completely determined task. There is no fermion operator
which could be identified with the number operator of a particular pair. Nev-
evertheless, three possibilities have been investigated in the present paper how
to get quantities that may be related to the pair numbers. Though methods
give different results, two important conclusions of Ref. [1] remain unchanged.
Namely, the odd-even staggering in pair numbers in even-even and odd-odd
$N = Z$ nuclei and the reduction of the np-pair number with increasing $T_z$ are
observed in all three procedures. The boson counting method seems to have
certain advantages as it obeys the natural relations (3) and (4) for pair num-
bers and gives a zero pair number for the particular pairing mode switched off
in the Hamiltonian.

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