Proton-neutron pairing effects in medium and heavy mass nuclei

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The consistency of the BCS approach in treating proton-neutron pairing correlations is examined. Generalized BCS transformations, which combine proton and neutron states, are used to extract the pairing gap parameter. This procedure gives energy gains due to the inclusion of proton-neutron pairing correlations, but the effect is found to be restricted to small values of the neutron excess $(N-Z)$. [S0556-2813(97)06708-3]

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The study of pairing correlations in finite nuclei has been the subject of many efforts. For a review of the problem the reader is referred to Goodman's review article [1]. Recently, interest in the study of the interplay between different channels of the pairing interaction has been renewed, particularly, after the findings of Engel *et al.* [2] and Satula and Wyss [3] about the balance between isovector and isoscalar components of the interaction. The treatment of proton-neutron pairing correlations was found to be relevant, also, for the description of alpha-decay [4] and double-beta-decay studies [5,6].

Generalized gap equations have been obtained by Goodman [7] which include $T=0$ and $T=1$ pairing correlations in the description of $N=Z$ nuclei in the s-d shell. In the work of [7] the need for a self-consistent HFB calculation was emphasized and the correspondence between this treatment and the method of Goswami [8] and Goswami and coworkers [9] was established. Concerning the case of $N\neq Z$ nuclei, the approach of [7] leads to an almost negligible contribution of proton-neutron ($T=1$) correlations in time-reversed orbitals.

The effect of proton-neutron pairing correlations in heavy-mass nuclei was studied by Delion *et al.* [4] in dealing with the calculation of alpha-decay observables. In the work of [4] the effect of proton-neutron pairing in the $T=1$ channel was found to be of minor importance and it was shown that a renormalization of the proton-proton and neutron-neutron pairing correlations could be used to account for proton-neutron pairing effects.

At variance with the results of [7] and [4] the calculations reported by Cheoun *et al.* [5] and by Pantis *et al.* [6] seemingly assigned a major role to proton-neutron pairing effects in medium-mass and heavy-mass nuclei. The inclusion of these correlations, accordingly to [5] and [6], leads to dramatic changes in the matrix elements for two-neutrino and neutrinoless modes of nuclear double-beta decay.

The connection between pairing and isospin symmetry in proton-rich nuclei was suggested by Engel *et al.* [2]. In the work of [2] the $T=1$ channel of the pairing interaction has been calculated in a senioritylike model and it was found that there exists an interplay between like-particle and unlike-particle components of the isovector pairing, near $N=Z$. In [2] the analogies exhibited by the features found in schematic model calculations [10,11] and by those of realistic shell-model calculations have been pointed out.

Although the study of pn-pairing correlations is by now more than 20 years old, some questions are still open, like the dependence of these correlations on the neutron (or proton) excess, the asymmetry between single-particle orbits, and the symmetry breaking induced by the renormalization of the pairing coupling constants. Also, the question of the suitability of the BCS transformation to account for the mixing between different pairing correlations is still open. While some authors have advocated in favor of it [9] others [7] have strongly opposed it, thus leaving a contradictory view of the problem.

In the present work we concentrate on the calculation of proton-neutron pairing correlations in time-reversed states with $J=0$, which correspond to proton-proton, neutron-neutron, and proton-neutron $T=1$ correlations. The resulting $T=1$ pairing-contributions are computed in this subspace, where the breaking of the isospin symmetry is enforced by a renormalization of the pairing coupling constant for unlike (proton-neutron) pairs. We have performed generalized BCS transformations for several nuclei with increasing neutron excess. The equations, on which the formalism is based, were also solved for the case of a single-shell model space [10,11]. By performing a boson expansion due to Evans and Krauss [12] the exact solution of the Hamiltonian in the single-shell basis is compared to the approximate BCS one.

A brief review of the formalism is presented in the following section, where the generalized BCS formalism and an exactly solvable model are introduced. We then discuss the results of the calculations, corresponding to various isotopes of the nuclei Ni, Zn, Ge, Se, Te, and Xe.

In the following, we shall briefly introduce the equations which we have solved to describe proton-neutron (pn) pairing correlations in time-reversed orbits. The formalism is well known and the details can be found in [8] and in [9]. The starting pairing Hamiltonian is written as

$$H=\sum_{jmt}\epsilon_{jt}a^{\dagger}_{jmt}a_{jmt}-\frac{1}{4}\sum_{jmj'm'}\sum_{tt'}G_{tt'}a^{\dagger}_{jmt}a^{\dagger}_{\overline{jmt'}}a_{\overline{j'm't'}}a_{j'm't},\qquad(1)$$

where the index (jmt) represents the angular momentum, its

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projection, and the isospin projection of the single-particle (s.p.) state created (annihilated) by the operator $a^{\dagger}(a)$; $G_{tt'}$ are the coupling constants of the separable monopole pairing interaction.

The pn BCS transformations have been applied to the $T=1$ component of the Hamiltonian (1).

In analogy to the case of light-mass ($N=Z$) nuclei [7] the pn BCS transformation [9] reads

$$\begin{pmatrix} c_{j1}^{\dagger} \\ c_{j2}^{\dagger} \\ c_{\overline{j1}} \\ c_{\overline{j2}} \end{pmatrix} = \begin{pmatrix} u_{11j} & u_{12j} & v_{11j} & v_{12j} \\ u_{21j} & u_{22j} & v_{21j} & v_{22j} \\ -v_{11j} & -v_{12j} & u_{11j} & u_{12j} \\ -v_{21j} & -v_{22j} & u_{21j} & u_{22j} \end{pmatrix} \begin{pmatrix} a_{jp}^{\dagger} \\ a_{jn}^{\dagger} \\ a_{\overline{jp}} \\ a_{\overline{jn}} \end{pmatrix}, \quad (2)$$

where for simplicity we have denoted by (j) the full set of quantum numbers which are needed to define a s.p. orbit and by (p) or (n) the corresponding isospin projections for protons and neutrons, respectively. The elements $u_{ik,j}$ and $v_{ik,j}$ of this transformation are constrained by anticommutation relations and the transformation is unitary. The above introduced 4×4 BCS matrix is just the limit of the generalized (complex) 8×8 transformation of Ref. [7] for vanishing $T=0$ interactions [9].

After some algebra, the transformed Hamiltonian can be written as the sum of a constant term (H_0), a linear term in the generalized quasiparticle operators (H_{11}), and a pair creation (annihilation) term (H_{20}). The solutions for the coefficients of the pn BCS transformation are obtained by imposing the fulfillment of the number and gap equations. As pointed out in [7] the fact that one can find a solution does not uniquely determine a set of physical values for the parameters of the pn BCS transformation. In order to guarantee the physical meaning of a solution we have calculated the values of H_0 and H_{20} and checked the consistency of H_{11} for each set of parameters u and v. Physical solutions are restricted only to those leading to the smallest value of H_0 and to a vanishing value of H_{20}. In order to grasp the main features of the solutions which are obtained by using the above-described formalism, we shall briefly introduce an exactly solvable model [10].

The Hamiltonian of this solvable model corresponds to the one-shell limit of Eq. (1). The single-j basis includes two Ω substates, herewith denoted by the index k, and in this basis the Hamiltonian (1) reduces to

$$H=-G_{pp}A_p^{\dagger}A_p-G_{nn}A_n^{\dagger}A_n-G_{pn}A_{pn}^{\dagger}A_{pn}. \quad (3)$$

The definition of the pair operators A is given in [12]. Together with the generators of the SU(2) group (isospin) and the number operators, these pair operators form the algebra of the Sp(4) group [10,11]. The solution of the Hamiltonian (3) can be obtained by using the techniques developed long ago by Hetch [10] and more recently used by Engel *et al.* [2]. An alternative way of solving this Hamiltonian consists of transforming it to a boson basis, by following the method introduced by Evans and Krauss [12]. After expand-

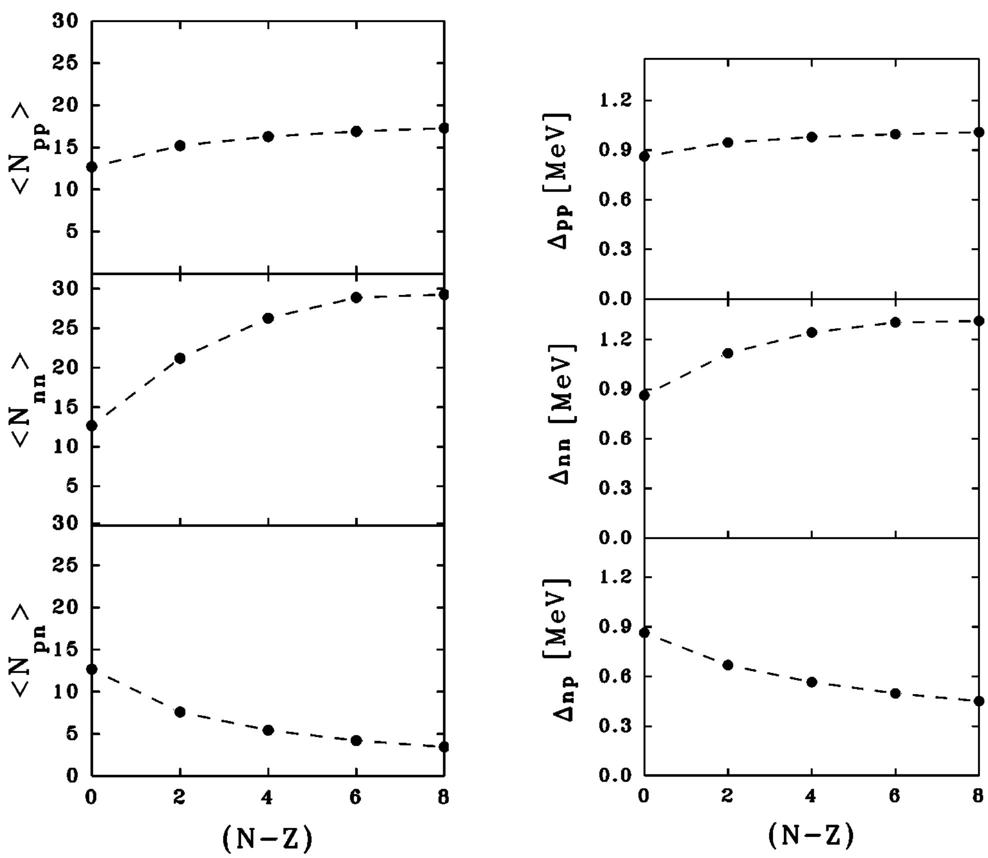

FIG. 1. Number of proton pairs (N_{pp}), neutron pairs (N_{nn}), and proton-neutron pairs (N_{pn}), as a function of the difference between the number of neutrons (N) and protons (Z), for the exactly solvable model discussed in the text and the corresponding gaps.

TABLE I. Values of the BCS pairing correlation energy $[E_0 = E_0(\Delta \neq 0) - E_0(\Delta = 0)]$ for the isotopes ^{60,62,64,66,68}Zn. The neutron-proton number difference $(N-Z)$ is given in the first column, and the values of E_0 without ($G_{pn}=0$) and with ($G_{pn}\neq 0$) pn correlations are shown as case (a) and case (b), respectively. The corresponding values of the adopted pairing coupling constants are $G_{pp}=G_{nn}=20/A$ MeV, $G_{pn}=26/A$ MeV, respectively.

$N-Z$	E_0 (a)	E_0 (b)
0	−4.198	−6.373
2	−5.640	−7.028
4	−6.331	−6.930
6	−6.348	−6.348
8	−5.956	−5.956

ing the operators which appear in Eq. (3) in terms of boson operators and introducing the states

$$|sn_fN_pN_n\rangle = \frac{1}{\sqrt{n_f!(N_p-s-n_f)!(N_n-s-n_f)!}} \times b_f^{\dagger n_f} b_p^{\dagger (N_p-s-n_f)/2} b_n^{\dagger (N_n-s-n_f)/2} |\rangle, \tag{4}$$

where s represents the seniority of the irreducible representation of Sp(4) [10] and the matrix elements of the Hamiltonian (3) are calculated.

Following the method of [2] one can estimate the number of like-particle pairs (neutron-neutron and proton-proton pairs) and unlike-particle pairs (proton-neutron pairs) by computing the expectation value of the operators

$$N_{np}=A_{pn}^{\dagger}A_{pn}, \quad N_{pp}=A_p^{\dagger}A_p, \quad N_{nn}=A_n^{\dagger}A_n. \tag{5}$$

The corresponding gap parameters are given by

$$\Delta_{np}=G_{pn}\sqrt{\langle N_{pn}\rangle}, \quad \Delta_{pp}=G_{pp}\sqrt{\langle N_{pp}\rangle}, \quad \Delta_{nn}=G_{nn}\sqrt{\langle N_{nn}\rangle}, \tag{6}$$

respectively.

TABLE II. Same as Table I, for ^{64,66,68,70,72,74,76}Ge with $G_{pp}=G_{nn}=16/A$ MeV and $G_{pn}=20/A$ MeV.

$N-Z$	E_0 (a)	E_0 (b)
0	−8.762	−14.738
2	−8.673	−12.167
4	−7.386	−8.754
6	−4.099	−4.099
8	−4.404	−4.404
10	−6.506	−6.506
12	−6.905	−6.905

The results of the above-introduced formalism, for the case of a single-j shell (with $\Omega=10$), are shown in Fig. 1. As described in the previous section, these are the expectation values $\langle N_{np}\rangle$, $\langle N_{pp}\rangle$, and $\langle N_{nn}\rangle$ of the operators given in Eq. (5). As shown in this figure, the proton-neutron pair correlations are strongly dependent on the difference between the number of neutrons and protons, as pointed out in [2]. For $N=Z$ the expectation values are similar but a strong suppression of the number of pn pairs is obtained, even for a relatively small value of the difference $N-Z$ ($N-Z=2$). For values of ($N-Z>4$) the number of pn pairs saturates. This result seemingly suggests that a renormalization of the other channels (pp and nn) can be introduced in order to include proton-neutron pairing interactions, as done in [4].

Concerning the question of the persistence of this trend in a realistic case, with open shells both for neutrons and protons, we shall discuss next the results of the pn BCS transformation, for several medium and heavy mass nuclei. The single-particle basis used in the calculations corresponds to an effective harmonic oscillator central potential, with Nilsson single-particle energies. For each of the considered cases the coefficients of the BCS transformation have been determined self-consistently. Each solution was then used to compute the value of the pairing correlation energy. The results corresponding to isotopes of Zn and Ge are shown in Tables I and II.

In the calculations, the coupling constant for pn pairing channels differs from the coupling constant used for proton-

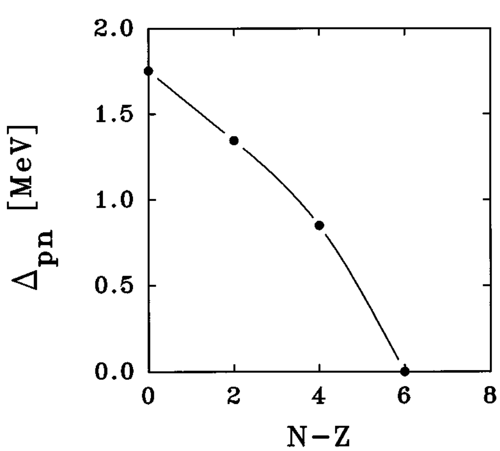

FIG. 2. Self-consistent proton-neutron pairing gap Δ_{pn}, as a function of $(N-Z)$, for the isotopes of Ni and with $G_{nn}=G_{pp}=24/A$ MeV and $G_{pn}=28/A$ MeV.

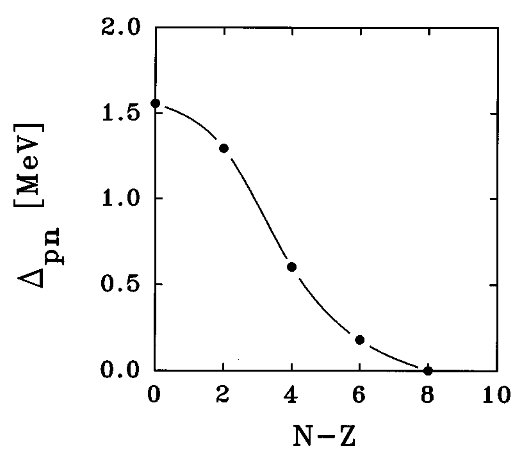

FIG. 3. Self-consistent proton-neutron pairing gap Δ_{pn}, as a function of $(N-Z)$, for the isotopes of Se and with $G_{nn}=G_{pp}=16/A$ MeV and $G_{pn}=20/A$ MeV.

proton and neutron-neutron pairing correlations. This is an important fact because the pure like-particle (proton-proton and neutron-neutron) solution always dominates if the pn coupling is not renormalized.

As seen in these tables, the energy gain due to pn pairing correlations vanishes for values of $N-Z>4$. For the cases of the isotopes of Te and Xe no energy gain has been obtained by including pn pairing correlations.

The values of Δ_{pn}, for some of the nuclei considered, are shown in Figs. 2 and 3. The similarities between the results of the exactly solvable model (Fig. 1) and the realistic cases are evident. This is in agreement with the findings of Refs. [2–4].

In contrast to the results shown in Figs. 1–3, the treatment of [5] leads to a completely different conclusion about the importance of pn pairing correlations. The method used by [5] mixes up $T=0$ and $T=1$ channels of the interaction and fixes the proton-neutron pairing gap. The solutions which are obtained in this way could lead to an abnormal enhancement of the proton-neutron mixing, as we have seen from the results of our calculations.

In summary, the question of the magnitude of proton-neutron pairing correlations and their influence on the total pairing energy and BCS occupation factors has been discussed, in this work, by using a pn BCS transformation. The results of this treatment show that pn pairing in time-reversed orbits does not seriously affect the properties of medium mass nuclei, except for very low values of the neutron excess $N-Z$. However, no gain in energy is obtained for heavy mass nuclei (Te, Xe). These results, for the nuclei which we have considered, are similar to the ones corresponding to the exactly solvable model of [2]. The consistency of the present approach was tested by using a boson expansion technique. The agreement between the results of [2] and the present ones, for a restricted configuration space, was shown based on the results obtained by using this boson expansion method. The effects of asymmetries in the proton and neutron single-particle energies and the breaking of the isospin symmetry, by renormalization of the coupling constants G_{nn}, G_{pp}, and G_{pn}, as well as a comparison between BCS and shell-model results are studied in [13].

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