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RESEARCH

Number projected isovector neutron–proton pairing effect in odd-mass nuclei

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Abstract A formalism which enables one to strictly conserve the number of particles when taking into account the isovector pairing correlations is presented in the case of odd-mass nuclei. With this aim, we had to first establish the expression of the projector for such systems. Expressions of the ground state and its energy have been exhibited. The model has been numerically tested in the framework of a schematic model.

Keywords Neutron–proton pairing · Particle-number projection · Odd-mass nuclei

Background

During the past two decades, many works have been devoted to the study of neutron–proton (np) pairing correlations (see, e.g. [1–17]). Indeed, the region of $N \simeq Z$ medium mass nuclei is now accessible to experiments and this fact led to renewed interest of theoreticians for this kind of nuclei. In the latter, one expects that neutrons and protons occupy the same levels and thus that the np pairing effect would be important. This effect is often treated within the BCS approximation [1–8]. However, it is well known that the major defect of the BCS theory is its violation of the particle-number conservation symmetry, in the pairing between like-particles case [18–22] as well as in the np pairing case.

The particle-number symmetry may be restored using a projection method. Several methods have been already proposed in the np pairing case, as the quasiparticle random phase approximation (QRPA) [23–31], the Lipkin-Nogami method [32], the generator coordinate method [33], and the PBCS-type projection methods [34], of FBCS-type [35] or the isospin and particle-number projection one [36]. In previous papers [37–40], we proposed and applied a generalization of the SBCS (sharp-BCS) projection method [41–43]. However, this generalization is valid only for even–even nuclei and has not been yet extended to odd-mass systems. The goal of the present work is to propose a formalism which could be applied to odd-mass nuclei. It is based on the Wahlborn blocking method [44, 45].

For a seek of coherence, the method for the diagonalization of the Hamiltonian and the BCS formalism are recalled in the first two sections. The particle-number conservation method is then presented in the next section. The formalism is numerically applied to a schematic model in the 'Numerical results and discussion' section. Main conclusions are summarized in last section.

Hamiltonian: diagonalization

Let us consider a system constituted by N neutrons and Z protons. In the second quantization and isospin formalism, the Hamiltonian which describes this system is given, in the isovector pairing case, by [5], [8]:

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$$\mathbf{H} = \sum_{\nu>0,t} \varepsilon_{\nu t}(a^+_{\nu t}a_{\nu t} + a^+_{\tilde{\nu}t}a_{\tilde{\nu}t}) - \frac{1}{2}\sum_{tt'} G_{tt'} \sum_{\nu,\mu>0} (a^+_{\nu t}a^+_{\tilde{\nu}t'}a_{\tilde{\mu}t'}a_{\mu t} + a^+_{\nu t}a^+_{\tilde{\nu}t'}a_{\tilde{\mu}t}a_{\mu t'}), \tag{1}$$

where the subscript t corresponds to the isospin component ($t = n, p$) and $a^+_{\nu t}$ and $a_{\nu t}$, respectively, represent the creation and annihilation operators of the particle in the state $|\nu t\rangle$, of energy $\varepsilon_{\nu t}$; $|\widetilde{\nu} t\rangle$ is the time-reverse of $|\nu t\rangle$ and $G_{tt'}$ characterizes the pairing-strength (one assumes that $G_{tt'}$ is constant and $G_{np} = G_{pn}$). The neutrons and protons are supposed to occupy the same energy levels.

In order to conserve, on average, the number of particles (i.e. neutrons and protons), let us introduce the Lagrange parameters λ_t ($t = n, p$) and diagonalize the auxiliary Hamiltonian

$$\mathbf{H} - \sum_t \lambda_t \mathbf{N}_t, \tag{2}$$

where $\mathbf{N}_t$ are the particle-number operators given by

$$\mathbf{N}_t = \sum_{\nu>0}\left(a^+_{\nu t}a_{\nu t} + a^+_{\widetilde{\nu t}}a_{\widetilde{\nu t}}\right), \quad t = n, p \tag{3}$$

Using the Wick theorem, the linearized part of the auxiliary Hamiltonian (2), denoted $\mathbf{H}'$, may be written, in a matricial form:

$$\mathbf{H}' = E_0 + \sum_{\nu>0,t}\xi_{\nu t} + \sum_{\nu>0}\begin{pmatrix} a^+_{\nu p} & a^+_{\nu n} & a_{\tilde{\nu}p} & a_{\tilde{\nu}n}\end{pmatrix} A_\nu \begin{pmatrix} a_{\nu p} \\ a_{\nu n} \\ a^+_{\tilde{\nu}p} \\ a^+_{\tilde{\nu}n}\end{pmatrix}, \tag{4}$$

where E_0 is the constant term, A_ν is the excitation matrix given by

$$A_\nu = \begin{pmatrix} \xi_{\nu p} & 0 & -\Delta_{pp} & -\Delta_{np} \\ 0 & \xi_{\nu n} & -\Delta_{np} & -\Delta_{nn} \\ -\Delta_{pp} & -\Delta_{np} & -\xi_{\nu p} & 0 \\ -\Delta_{np} & -\Delta_{nn} & 0 & -\xi_{\nu n}\end{pmatrix} \tag{5}$$

and where we set:

$$\xi_{\nu t} = \tilde{\varepsilon}_{\nu t} - \frac{1}{2}\sum_r G_{rt}(1+\delta_{rt})\overline{a^+_{\tilde{\nu}t}a_{\tilde{\nu}t}}, \quad \tilde{\varepsilon}_{\nu t} = (\varepsilon_{\nu t} - \lambda_t) \tag{6}$$

and

$$\Delta_{tt'} = G_{tt'}\sum_{\nu>0}\overline{a^+_{\nu t}a^+_{\tilde{\nu}t'}} = G_{tt'}\sum_{\nu>0}\overline{a_{\tilde{\nu}t}a_{\nu t'}} \tag{7}$$

Using the generalized Bogoliubov–Valatin transformation

$$\begin{cases} \alpha^+_{\nu\tau} = \sum_{t=n,p}(u_{\nu\tau t}a^+_{\nu t} + v_{\nu\tau t}a_{\tilde{\nu}t}) \\ \alpha_{\nu\tau} = \sum_{t=n,p}(u_{\nu\tau t}a_{\nu t} + v_{\nu\tau t}a^+_{\tilde{\nu}t}) \end{cases} \quad \tau = 1, 2 \tag{8}$$

the Hamiltonian (4) becomes

$$\mathbf{H}' = E_0 + \sum_{\nu>0,t}\xi_{\nu t} + {}^tV\begin{pmatrix} E_{\nu 1} & 0 & 0 & 0 \\ 0 & E_{\nu 2} & 0 & 0 \\ 0 & 0 & -E_{\nu 1} & 0 \\ 0 & 0 & 0 & -E_{\nu 2}\end{pmatrix}V$$

with the notations

$$E^2_{\nu\tau} = \frac{1}{2}\left[\left(E^2_{\nu p} + E^2_{\nu n} + 2\Delta^2_{np}\right) + (-1)^\tau\sqrt{R_\nu}\right], \quad \tau = 1, 2$$

$$R_\nu = \left(E^2_{\nu p} - E^2_{\nu n}\right)^2 + 4\Delta^2_{np}\left[E^2_{\nu p} + E^2_{\nu n} - 2\left[\xi_{\nu n}\xi_{\nu p} - \Delta_{nn}\Delta_{pp}\right]\right]$$

$$E^2_{\nu t} = \xi^2_{\nu t} + \Delta^2_{tt}, \quad t = n, p$$

$$V = \begin{pmatrix} \alpha_{\nu 1} \\ \alpha_{\nu 2} \\ \alpha^+_{\tilde{\nu}1} \\ \alpha^+_{\tilde{\nu}2}\end{pmatrix}$$

BCS formalism

Ground state

The BCS ground state is obtained by eliminating all the quasiparticles from the actual vacuum, i.e. $|\Psi\rangle \propto \prod_{\nu,\tau}\alpha_{\nu\tau}|0\rangle$.

Using the Bogoliubov–Valatin transformation (8), this state may be written, after normalization, in the particle representation:

$$|\Psi\rangle = \prod_{j>0}|\Psi_j\rangle \tag{9}$$

with

$$|\Psi_j\rangle = \left[B^j_1 A^+_{jp}A^+_{jn} + B^j_p A^+_{jp} + B^j_n A^+_{jn} + B^j_4\left(a^+_{\widetilde{jp}}a^+_{jn} + a^+_{\widetilde{jn}}a^+_{jp}\right) + B^j_5\right]|0\rangle, \tag{10}$$

where $A^+_{jt} = a^+_{\widetilde{jt}}a^+_{jt}$ refers to the creation operator of a particle pair.

However, the state (9) can only describe even–even systems since it is a superposition of even states. For an even–odd system, if one assumes that the blocked level is νT ($T = n$ or p), the ground state is given by [46, 47]

$$|\nu T\rangle = a^+_{\nu T}\prod_{\substack{j>0 \\ j\neq\nu}}|\Psi_j\rangle, \tag{11}$$

where $|\Psi_j\rangle$ is defined by (10).

It is worth noticing that in the latter expression, the coefficients B^j_i that appear in (10) depend on ν; this dependence has not been explicited in order to simplify the notations.

Let us note that the limits when $\Delta_{np} \to 0$ of all expressions in the np pairing case are given in "Appendix A".

Gap equations—Energy

Even–even system

The gap equations, as well as the energy expression, are well established in the framework of the BCS formalism for an even–even system. In the following, we will briefly recall them so as to show later the differences with the even–odd systems.

The total particle-number operator is defined by $\mathbf{N} = \sum_t \mathbf{N}_t$. Using Eq. (9), the particle-number conservation condition reads:

$$\langle \Psi|\mathbf{N}|\Psi\rangle = 2\sum_{j>0}\left[2(B_1^j)^2 + \left(B_p^j\right)^2 + (B_n^j)^2 + 2\left(B_4^j\right)^2\right] \quad (12)$$

In the same way, the gap parameters defined by (7) become

$$\Delta_{tt} = -G_{tt}\sum_{j>0}\left(B_1^jB_t^j + B_5^jB_{t'}^j\right) \quad (t = n, p, \quad t' \neq t)$$
$$\Delta_{np} = -G_{np}\sum_{j>0}B_4^j\left(B_1^j - B_5^j\right) \quad (13)$$

Finally, the system energy is given by

$$E_0 = 2\sum_{j>0}\left\{\left[(B_1^j)^2 + \left(B_4^j\right)^2\right](\varepsilon_{jp} + \varepsilon_{jn}).\right.$$
$$+\sum_t\left[\left(B_t^j\right)^2\varepsilon_{jt} - \frac{1}{2}G_{tt}\left((B_1^j)^2 + \left(B_t^j\right)^2\right)\right]$$
$$\left.-\frac{1}{2}G_{np}\left[(B_1^j)^2 + 2\left(B_4^j\right)^2\right]\right\}$$
$$-\sum_{\substack{j,l>0\\ j\neq l}}\left\{\sum_t G_{tt}\left(B_1^jB_{t'}^j + B_t^jB_5^j\right)\left(B_1^lB_{t'}^l + B_t^lB_5^l\right)\right.$$
$$\left.+2G_{np}B_4^j\left(B_1^j - B_5^j\right)B_4^l\left(B_1^l - B_5^l\right)\right\}, \quad (14)$$

where $t' \neq t$ (i.e. $t' = n(p)$ if $t = p(n)$).

Even–odd system

In the case of an even–odd system, the particle-number conservation condition reads, using the state (11)

$$\langle \nu T|\mathbf{N}|\nu T\rangle = 1 + 2\sum_{\substack{j>0\\ j\neq\nu}}\left[2(B_1^j)^2 + \left(B_p^j\right)^2 + (B_n^j)^2 + 2\left(B_4^j\right)^2\right] \quad (15)$$

As for the gap parameters, they are given by

$$\Delta_{tt}^{(\nu)} = -G_{tt}\sum_{\substack{j>0\\ j\neq\nu}}\left(B_1^jB_t^j + B_5^jB_{t'}^j\right) \quad (t = n, p, \quad t' \neq t)$$
$$\Delta_{np}^{(\nu)} = 2G_{np}\sum_{\substack{j>0\\ j\neq\nu}}B_4^j\left(B_1^j - B_5^j\right) \quad (16)$$

The system energy is given, in this case, by

$$E_0^{\nu T} = \varepsilon_{\nu T} + 2\sum_{\substack{j>0\\ j\neq\nu}}\left\{\left[(B_1^j)^2 + \left(B_4^j\right)^2\right](\varepsilon_{jp} + \varepsilon_{jn}).\right.$$
$$+\sum_t\left[\left(B_t^j\right)^2\varepsilon_{jt} - \frac{1}{2}G_{tt}\left((B_1^j)^2 + \left(B_t^j\right)^2\right)\right]$$
$$\left.-\frac{1}{2}G_{np}\left[(B_1^j)^2 + 2\left(B_4^j\right)^2\right]\right\}$$
$$-\sum_{\substack{j,l>0\\ j\neq l\neq\nu}}\left\{\sum_t G_{tt}\left(B_1^jB_{t'}^j + B_t^jB_5^j\right)\left(B_1^lB_{t'}^l + B_t^lB_5^l\right)\right.$$
$$\left.+2G_{np}B_4^j\left(B_1^j - B_5^j\right)B_4^l\left(B_1^l - B_5^l\right)\right\}, \quad (17)$$

where $t' \neq t$. Expressions (15–17) are similar to their homologues (12–14) of the even–even case. One can clearly see that the blocked level is occupied by the single particle and that the index ν is excluded from the summations over j.

Particle-number projection

Ground state

It is well established that the states (9) and (11) are not eigenstates of the particle-number operator. However, the particle-number symmetry may be restored using a particle-number projection method. In the present work, we use the sharp-BCS (SBCS) one [37–40].

Even–even system

The operator that enables one to project the conventional BCS state (i.e. in the pairing between like-particles case) on the good particle number is given by [45]:

$$\mathcal{P} = \frac{1}{2\pi}\int_0^{2\pi}\exp(i\varphi(\mathbf{N} - 2P))\mathrm{d}\varphi \quad (18)$$

P being the number of pairs of particles and $\mathbf{N}$ the particle-number operator of the considered system.

Its discrete form is given by [42]

$$\mathcal{P}_m = \frac{1}{2(m+1)} \left\{ \sum_{k=0}^{m+1} \xi_k z_k^{-P} \prod_j \left[1 + a_j^+ a_j (\sqrt{z_k} - 1) \right] + c.c \right\}, \tag{19}$$

where:

$$z_k = \exp\left(\frac{ik\pi}{m+1}\right) \text{ and}$$

$$\xi_k = \left\{ \begin{array}{ll} \frac{1}{2} & \text{if } k = 0 \text{ or } k = m+1 \\ 1 & \text{otherwise} \end{array} \right\} \tag{20}$$

m is a non-zero integer which represents the extraction degree of the false components and "$c.c$" means the complex conjugate with respect to z_k.

In the isovector pairing case, the ground-state (9) is simultaneously projected on the good neutron and proton numbers, i.e. [38–40]:

$$\begin{aligned} |\Psi_{mm'}\rangle &= \mathcal{P}_n \mathcal{P}_p |\Psi\rangle \\ &= C_{mm'} \sum_{k=0}^{m+1} \sum_{k'=0}^{m'+1} \xi_k \xi_{k'} \left\{ z_k^{-P_N} z_{k'}^{-P_Z} |\Psi(z_k, z_{k'})\rangle, \right. \\ &\quad \left. + \bar{z}_k^{-P_N} z_{k'}^{-P_Z} |\Psi(\bar{z}_k, z_{k'})\rangle + c.c \right\} \end{aligned} \tag{21}$$

where

$$|\Psi(z_k, z_{k'})\rangle = \prod_{j>0} |\Psi_j(z_k, z_{k'})\rangle \tag{22}$$

with

$$\begin{aligned} |\Psi_j(z_k, z_{k'})\rangle = \Big\{ & z_k z_{k'} B_1^j A_{jp}^+ A_{jn}^+ + z_{k'} B_p^j A_{jp}^+ + z_k B_n^j A_{jn}^+ \\ & + \sqrt{z_k z_{k'}} B_4^j (a_{jp}^+ a_{\tilde{j}n}^+ + a_{\tilde{j}n}^+ a_{jp}^+) + B_5^j \Big\} |0\rangle \end{aligned} \tag{23}$$

$C_{mm'}$ is the normalization constant.

Even–odd system

In the pairing between like-particles case, for an odd system, constituted of $(2P+1)$ particles, the projector on the good particle-number is given by

$$\mathcal{P} = \frac{1}{2\pi} \int_0^{2\pi} \exp(i\varphi(\mathbf{N} - 2P - 1)) \mathrm{d}\varphi \tag{24}$$

Its discrete form is given by

$$\mathcal{P}_m = \frac{1}{2(m+1)} \left\{ \sum_{k=0}^{m+1} \xi_k z_k^{-(P+\frac{1}{2})} \prod_j \left[1 + a_j^+ a_j (\sqrt{z_k} - 1) \right] + c.c \right\} \tag{25}$$

One then obtains

$$\begin{aligned} |\nu T_{mm'}\rangle = C_{\nu mm'} \sum_{k=0}^{m+1} \sum_{k'=0}^{m'+1} \xi_k \xi_{k'} a_{\nu T}^+ \Big\{ & z_k^{-P_N} z_{k'}^{-P_Z} |\Psi(z_k, z_{k'})\rangle_\nu \\ & + \bar{z}_k^{-P_N} z_{k'}^{-P_Z} |\Psi(z_k, z_{k'})\rangle_\nu + c.c \Big\}, \quad T = n, p \end{aligned} \tag{26}$$

where

$$|\Psi(z_k, z_{k'})\rangle_\nu = \prod_{\substack{j>0 \\ j \neq \nu}} |\Psi_j(z_k, z_{k'})\rangle \tag{27}$$

$|\Psi_j(z_k, z_{k'})\rangle$ being defined by (9). Let us however recall that in this case the coefficients B_i^j depend on ν. $C_{\nu mm'}$ is the normalization constant.

Expectation values

Even–even system

The calculation of the expectation value of a given operator $\mathbf{O}$ that conserves the particle number is simplified by the use of the property [37]:

$$\langle \Psi_{mm'} | \mathbf{O} | \Psi_{mm'} \rangle = 4(m+1)(m'+1) C_{mm'} \langle \Psi | \mathbf{O} | \Psi_{mm'} \rangle \tag{28}$$

In particular, if $\mathbf{O}$ is the identity operator, the normalization condition of the wave-function (21) leads to

$$\begin{aligned} C_{mm'}^{-2} = 4(m+1)(m'+1) \sum_{k=0}^{m+1} \sum_{k'=0}^{m'+1} \xi_k \xi_{k'} \\ \times \Big\{ z_k^{-P_N} z_{k'}^{-P_Z} \prod_{j>0} A_j(z_k, z_{k'}) \\ + \bar{z}_k^{-P_N} z_{k'}^{-P_Z} \prod_{j>0} A_j(\bar{z}_k, z_{k'}) + c.c \Big\} \end{aligned} \tag{29}$$

with the notation

$$\begin{aligned} A_j(z_k, z_{k'}) = \Big\{ & z_k z_{k'} (B_1^j)^2 + z_{k'} (B_p^j)^2 + z_k (B_n^j)^2 \\ & + 2\sqrt{z_k z_{k'}} (B_4^j)^2 + (B_5^j)^2 \Big\} \end{aligned} \tag{30}$$

$\bar{z}_k$ being the complex conjugate with respect to z_k. P_N (respectively, P_Z) represents the number of pairs of neutrons (respectively, protons).

In the same way, the expectation value of the Hamiltonian (1) over the state $|\Psi_{mm'}\rangle$ reads

$$\begin{aligned} E_{mm'} = 4(m+1)(m'+1) C_{mm'}^2 \sum_{k=0}^{m+1} \sum_{k'=0}^{m'+1} \xi_k \xi_{k'} \\ \times \left[z_k^{-P_N} z_{k'}^{-P_Z} E(z_k, z_{k'}) + \bar{z}_k^{-P_N} z_{k'}^{-P_Z} E(\bar{z}_k, z_{k'}) + c.c \right] \end{aligned} \tag{31}$$

with

$$E(z_k, z_{k'}) = \sum_{j>0}\Big[E_0^j(z_k, z_{k'}) - G_{nn}E_n^j(z_{k'}) - G_{pp}E_p^j(z_k) - G_{np}E_{np}^j(z_k, z_{k'})\Big]\prod_{\substack{i>0\\ i\neq j}} A_i(z_k, z_{k'}) - \sum_{\substack{j,l>0\\ j\neq l}}\Big[G_{nn}z_k F_n^j(z_{k'})F_n^l(z_{k'}) + G_{pp}z_{k'}F_p^j(z_k)F_p^l(z_k) + 2G_{np}\sqrt{z_k z_{k'}}F_{np}^j(z_k, z_{k'})F_{np}^l(z_k, z_{k'})\Big]\prod_{\substack{i>0\\ i\neq j,l}} A_i(z_k, z_{k'}) \tag{32}$$

where

$$\begin{aligned}
E_0^j(z_k, z_{k'}) &= 2\Big\{\left(B_n^j\right)^2 z_k\varepsilon_{jn} + \left(B_p^j\right)^2 z_{k'}\varepsilon_{jp}. + \Big[\left(B_1^j\right)^2 z_k z_{k'} + \left(B_4^j\right)^2\sqrt{z_k z_{k'}}\Big]\left(\varepsilon_{jn}+\varepsilon_{jp}\right)\Big\}\\
E_n^j(z_{k'}) &= z_k\Big[\left(B_1^j\right)^2 z_{k'} + \left(B_n^j\right)^2\Big]\\
F_n^j(z_{k'}) &= B_1^j B_p^j z_{k'} + B_n^j B_5^j\\
E_p^j(z_k) &= z_{k'}\Big[\left(B_1^j\right)^2 z_k + \left(B_p^j\right)^2\Big]\\
F_p^j(z_k) &= B_1^j B_n^j z_k + B_p^j B_5^j\\
E_{np}^j(z_k, z_{k'}) &= \sqrt{z_k z_{k'}}\Big[\left(B_1^j\right)^2\sqrt{z_k z_{k'}} + 2\left(B_4^j\right)^2\Big]\\
F_{np}^j(z_k, z_{k'}) &= B_4^j\left(B_1^j\sqrt{z_k z_{k'}} - B_5^j\right),
\end{aligned} \tag{33}$$

and where $A_i(z_k, z_{k'})$ is given by Eq. (30).

The real parts of Eqs. (29) and (31) are given in "Appendix B".

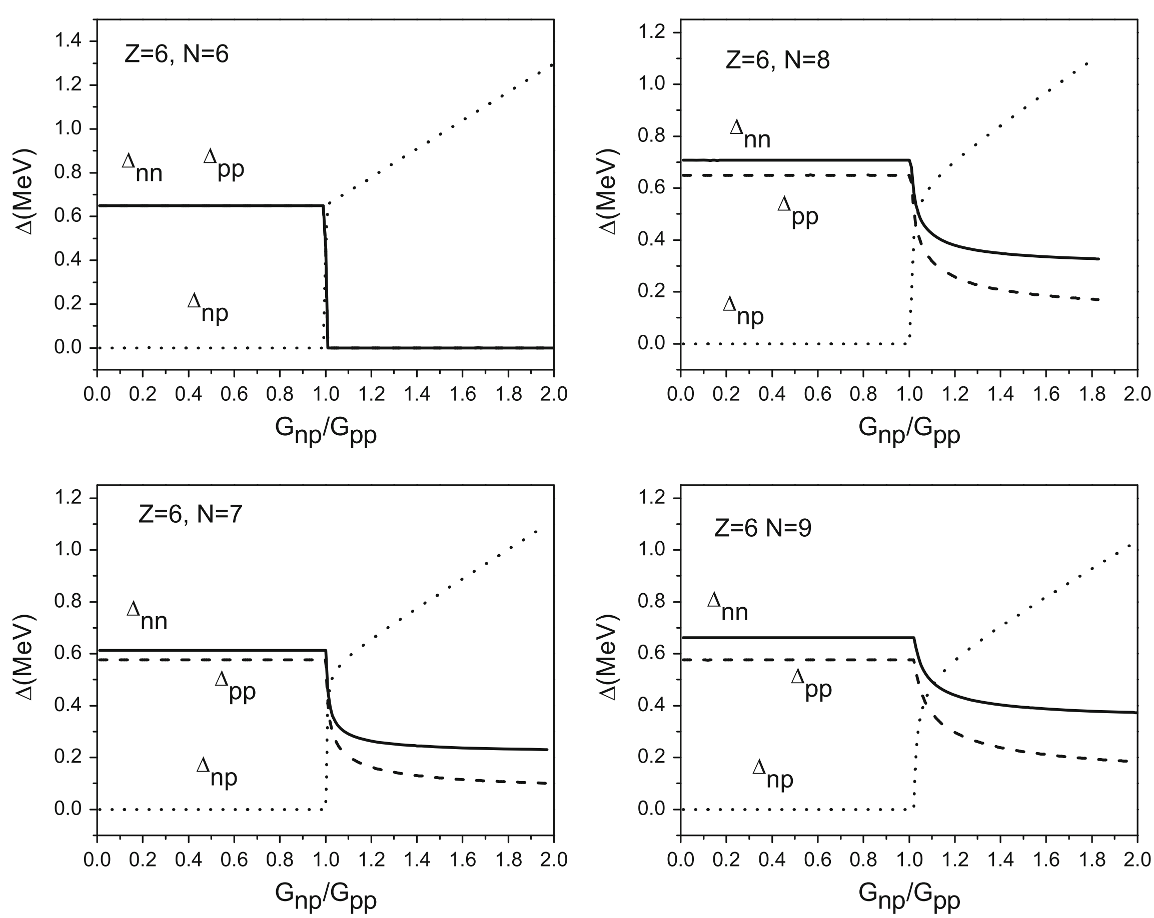

Fig. 1 Variation of the various gap parameters as a function of the ratio G_{np}/G_{pp} within the one-level model using $\Omega = 12$ and $G_{nn} = G_{pp} = 0.125$ MeV, for $Z = 6$ with $N - Z = 0, 1, 2, 3$

Even–odd system

In case of an even–odd system, using an expression similar to (28), one obtains for the normalization condition of the state (26):

$$C_{\nu mm'}^{-2} = 4(m+1)(m'+1)\sum_{k=0}^{m+1}\sum_{k'=0}^{m'+1}\xi_k\xi_{k'} \times \left\{ z_k^{-P_N} z_{k'}^{-P_Z} \prod_{\substack{j>0 \\ j\neq\nu}} A_j(z_k, z_{k'}) + \bar{z}_k^{-P_N} z_{k'}^{-P_Z} \prod_{\substack{j>0 \\ j\neq\nu}} A_j(\bar{z}_k, z_{k'}) + c.c \right\} \tag{34}$$

$A_j(z_k, z_{k'})$ being defined by (30).

The energy of the system is obtained using the wave-function (26), i.e.

$$E_{mm'}^{\nu T} = \varepsilon_{\nu T} + 4(m+1)(m'+1)C_{\nu mm'}^{2}\sum_{k=0}^{m+1}\sum_{k'=0}^{m'+1}\xi_k\xi_{k'} \times \left[z_k^{-P_N} z_{k'}^{-P_Z} E^{\nu}(z_k, z_{k'}) + \bar{z}_k^{-P_N} z_{k'}^{-P_Z} E^{\nu}(\bar{z}_k, z_{k'}) + c.c \right], \tag{35}$$

where we set

$$E^{\nu}(z_k, z_{k'}) = \sum_{\substack{j>0 \\ j\neq\nu}} \Big[E_0^j(z_k, z_{k'}) - G_{nn}E_n^j(z_{k'}) - G_{pp}E_p^j(z_k) - G_{np}E_{np}^j(z_k, z_{k'}) \Big] \prod_{\substack{i>0 \\ i\neq\nu}} A_i(z_k, z_{k'}) - \sum_{\substack{j,l>0 \\ j\neq l \\ j\neq\nu}} \Big(G_{nn} z_k F_n^j(z_{k'}) F_n^l(z_{k'}) + G_{pp} z_{k'} F_p^j(z_k) F_p^l(z_k) + 2G_{np}\sqrt{z_k z_{k'}} F_{np}^j(z_k, z_{k'}) F_{np}^l(z_k, z_{k'}) \Big) \prod_{\substack{i>0 \\ i\neq j,l \\ i\neq\nu}} A_i(z_k, z_{k'})$$

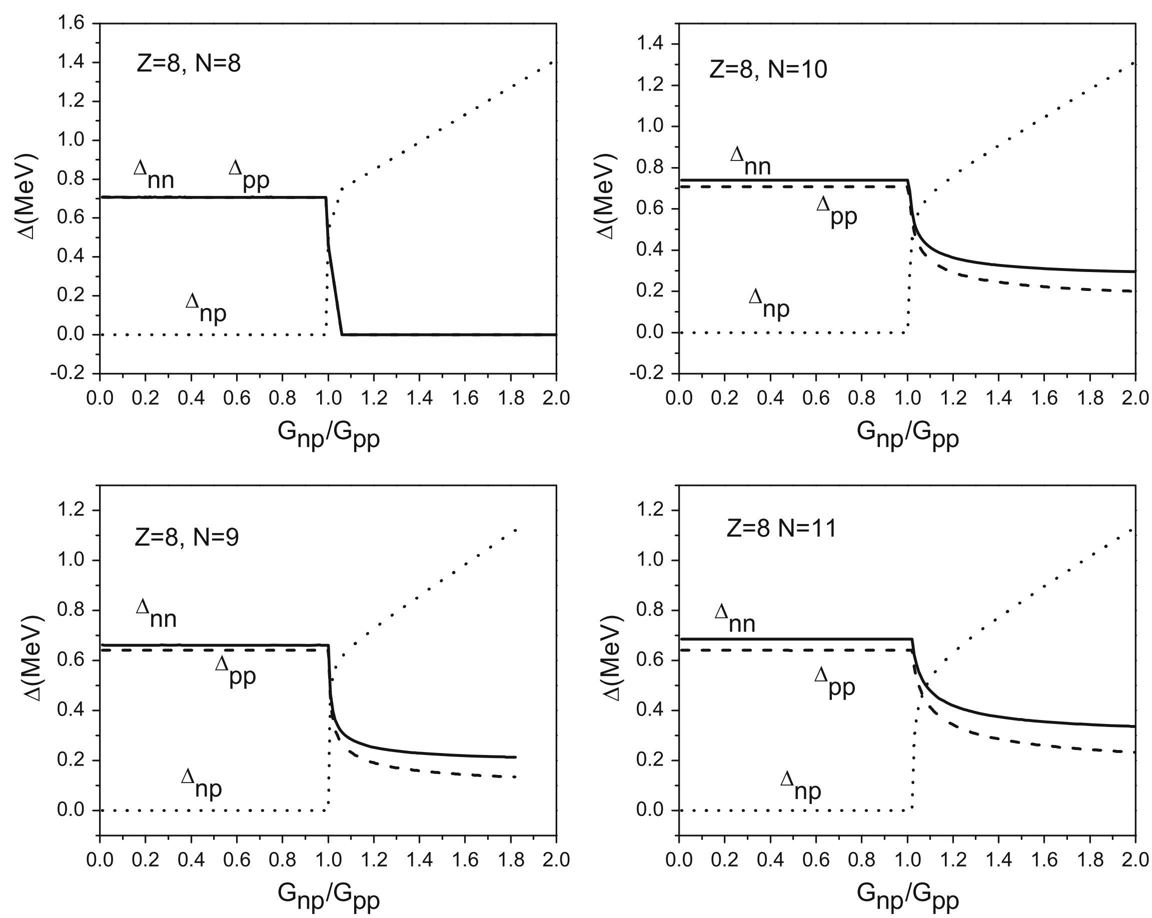

Fig. 2 Same as Fig. 1 for $Z = 8$ with $N - Z = 0, 1, 2, 3$

Table 1 Variation of the overlap between the projected and non-projected states, as a function of the extraction degrees of the false components, for an even–even system such as $Z = 6$, $N = 6$, $G_{pp} = 0.125$ MeV, $G_{nn} = 0.150$ MeV and $G_{np} = 0.137$ MeV

m	m'	$\langle \Psi \mid \Psi_{mm'} \rangle$	m	m'	$\langle \Psi \mid \Psi_{mm'} \rangle$
0	0	0.267	1	0	0.224
0	1	0.224	1	1	0.222
0	2	0.223	1	2	0.222
0	3	0.223	1	3	0.223
2	0	0.223	3	0	0.223
2	1	0.222	3	1	0.223
2	2	0.223	3	2	0.224
2	3	0.224	3	3	0.224

Table 2 Same as Table 1 for $Z = 8$, $N = 8$

m	m'	$\langle \Psi \mid \Psi_{mm'} \rangle$	m	m'	$\langle \Psi \mid \Psi_{mm'} \rangle$
0	0	0.268	1	0	0.217
0	1	0.217	1	1	0.216
0	2	0.216	1	2	0.216
0	3	0.216	1	3	0.216
2	0	0.216	3	0	0.216
2	1	0.217	3	1	0.217
2	2	0.217	3	2	0.217
2	3	0.217	3	3	0.217

Table 3 Variation of the overlap between the projected and non projected states, as a function of the extraction degrees of the false components, for an odd system such as $Z = 6, N = 7$, $G_{pp} = 0.125$ MeV, $G_{nn} = 0.150$ MeV and $G_{np} = 0.137$ MeV

m	m'	$\langle \nu T \mid \nu T_{mm'} \rangle$	m	m'	$\langle \nu T \mid \nu T_{mm'} \rangle$
0	0	0.249	1	0	0.195
0	1	0.195	1	1	0.189
0	2	0.195	1	2	0.189
0	3	0.194	1	3	0.189
2	0	0.197	3	0	0.198
2	1	0.189	3	1	0.189
2	2	0.190	3	2	0.190
2	3	0.190	3	3	0.190

Table 4 Same as Table 3 for $Z = 8$, $N = 9$

m	m'	$\langle \nu T \mid \nu T_{mm'} \rangle$	m	m'	$\langle \nu T \mid \nu T_{mm'} \rangle$
0	0	0.249	1	0	0.193
0	1	0.192	1	1	0.184
0	2	0.191	1	2	0.184
0	3	0.191	1	3	0.184
2	0	0.194	3	0	0.194
2	1	0.184	3	1	0.184
2	2	0.184	3	2	0.184
2	3	0.184	3	3	0.184

The terms $E_i^j(z_k, z_{k'})$, $F_i^j(z_{k'})$, $F_i^j(z_k)$ and $F_i^j(z_k, z_{k'})$ ($i = n, \ p, \ np$) are given by the same expressions as in the even–even case, i.e. by Eqs. (33). Let us note that the blocked particle does not contribute to the pairing energy, but its energy which is due to the occupation of the $|\nu\rangle$ level of the single-particles model appears in the total energy.

Numerical results and discussion

The previously described formalism has been tested within the schematic one-level model. In the latter, it is assumed that there is only one level of energy $\varepsilon_{\nu t} = 0 \, \forall \, \nu$ and for $t = n, p$. In all that follows, we used the total degeneracy of levels value $\Omega = 12$.

Gap parameters

We have first studied the variations of the various gap parameters as a function of the ratio G_{np}/G_{pp} in the even–even case as well as in the odd one. We used the values $Z = 6$ (see Fig. 1) and $Z = 8$ (see Fig. 2) with $(N - Z) = 0, 1, 2, 3$. In each case, the neutron and proton pairing-strength values are $G_{nn} = G_{pp} = 0.125$ MeV. The behavior of the Δ_{nn}, Δ_{pp} and Δ_{np} parameters in the even–even case (upper part of Figs. 1, 2) is similar to those of several works (see, e.g. References [3–5] and [7]). One notes that there exists a critical value of G_{np} (which will be hereafter denoted $\left(G_{np}\right)_c$), under which there is no np pairing (i.e. $\Delta_{np} = 0$ and the Δ_{nn} and Δ_{pp} values are those of the pairing between like-particles case).

In the odd case (lower part of Figs. 1, 2), the trends of the three curves are very similar to those of the even–even case, as underlined in References [46, 47].

Test of the projection method

In order to judge the efficiency of the projection method, we have studied the overlap between the BCS wave-function and the projected one in the even–even case ($\langle \Psi \mid \Psi_{mm'} \rangle$) (see Table 1 for $Z = 6$, $N = 6$ and Table 2 for $Z = 8$, $N = 8$) as well as in the odd one ($\langle \nu T \mid \nu T_{mm'} \rangle$) (see Table 3 for $Z = 6$, $N = 7$ and Table 4 for $Z = 8$, $N = 9$) as a function of the extraction degrees of the false components m and m'. We used in each case the values $G_{pp} = 0.125$ MeV, $G_{nn} = 0.150$ MeV and $G_{np} = 0.137$ MeV. One then notices a rapid convergence: in practice, the convergence is reached as soon as $m = m' = 3$ for all considered systems.

Table 5 Variation of the projected ground-state energy (in MeV) as a function of the extraction degrees of the false components, in the case of an even–even system such as $Z = 6$, $N = 6$, $G_{pp} = 0.125$ MeV, $G_{nn} = 0.150$ MeV and $G_{np} = 0.137$ MeV. The BCS energy is $E_0 = -7.733$ MeV

m'	m	$E_{mm'}$	m'	m	$E_{mm'}$
0	0	−7.780	1	0	−8.172
0	1	−8.168	1	1	−8.206
0	2	−8.161	1	2	−8.201
0	3	−8.163	1	3	−8.201
0	4	−8.164	1	4	−8.202
2	0	−8.165	3	0	−8.167
2	1	−8.201	3	1	−8.202
2	2	−8.200	3	2	−8.200
2	3	−8.200	3	3	−8.200
2	4	−8.200	3	4	−8.199
4	0	−8.169			
4	1	−8.202			
4	2	−8.200			
4	3	−8.199			
4	4	−8.199			

Table 6 Same as Table 5 for $Z = 8$, $N = 8$. The BCS energy is $E_0 = -9.349$ MeV

m'	m	$E_{mm'}$	m'	m	$E_{mm'}$
0	0	−9.431	1	0	−9.844
0	1	−9.838	1	1	−9.924
0	2	−9.837	1	2	−9.933
0	3	−9.837	1	3	−9.935
0	4	−9.837	1	4	−9.936
2	0	−9.843	3	0	−9.844
2	1	−9.933	3	1	−9.936
2	2	−9.936	3	2	−9.937
2	3	−9.936	3	3	−9.937
2	4	−9.937	3	4	−9.937
4	0	−9.844			
4	1	−9.937			
4	2	−9.937			
4	3	−9.937			
4	4	−9.937			

In addition, there exists an important discrepancy between the projected and non-projected states. Indeed, the overlap between the projected and non-projected wavefunctions is of the order of 0.22 for the even–even systems and of 0.19 for the odd ones. This shows the necessity of eliminating the false components of the BCS wavefunctions when calculating physical observables.

Table 7 Variation of the projected ground-state energy (in *MeV*) as a function of the extraction degrees of the false components, in the case of an odd system such as $Z = 6$, $N = 7$, $G_{pp} = 0.125$ MeV, $G_{nn} = 0.150$ MeV and $G_{np} = 0.137$ MeV. The BCS energy is $E_0^{\nu T} = -6.311$ MeV

m'	m	$E^{\nu T}_{mm'}$	m'	m	$E^{\nu T}_{mm'}$
0	0	−6.287	1	0	−7.353
0	1	−7.459	1	1	−7.544
0	2	−7.508	1	2	−7.555
0	3	−7.515	1	3	−7.560
0	4	−7.519	1	4	−7.561
2	0	−7.277	3	0	−7.259
2	1	−7.552	3	1	−7.555
2	2	−7.563	3	2	−7.566
2	3	−7.567	3	3	−7.569
2	4	−7.569	3	4	−7.571
4	0	−7.252			
4	1	−7.556			
4	2	−7.567			
4	3	−7.571			
4	4	−7.571			

Table 8 Same as Table 7 for $Z = 8$, $N = 9$. The BCS energy is $E_0^{\nu T} = -7.761$ MeV

m'	m	$E^{\nu T}_{mm'}$	m'	m	$E^{\nu T}_{mm'}$
0	0	−7.754	1	0	−8.551
0	1	−8.664	1	1	−8.832
0	2	−8.711	1	2	−8.875
0	3	−8.722	1	3	−8.881
0	4	−8.724	1	4	−8.884
2	0	−8.559	3	0	−8.549
2	1	−8.878	3	1	−8.880
2	2	−8.886	3	2	−8.889
2	3	−8.889	3	3	−8.892
2	4	−8.891	3	4	−8.893
4	0	−8.545			
4	1	−8.881			
4	2	−8.890			
4	3	−8.893			
4	4	−8.893			

Energy

We have first studied the convergence of the method for the projected ground-state energy. As it can be seen in Tables 5 and 6 (respectively, Tables 7 and 8) where we reported the variations of $E_{mm'}$ (respectively, $E^{\nu T}_{mm'}$) as a function of the extraction degrees of the false components m and m', in the case of even–even systems (respectively,

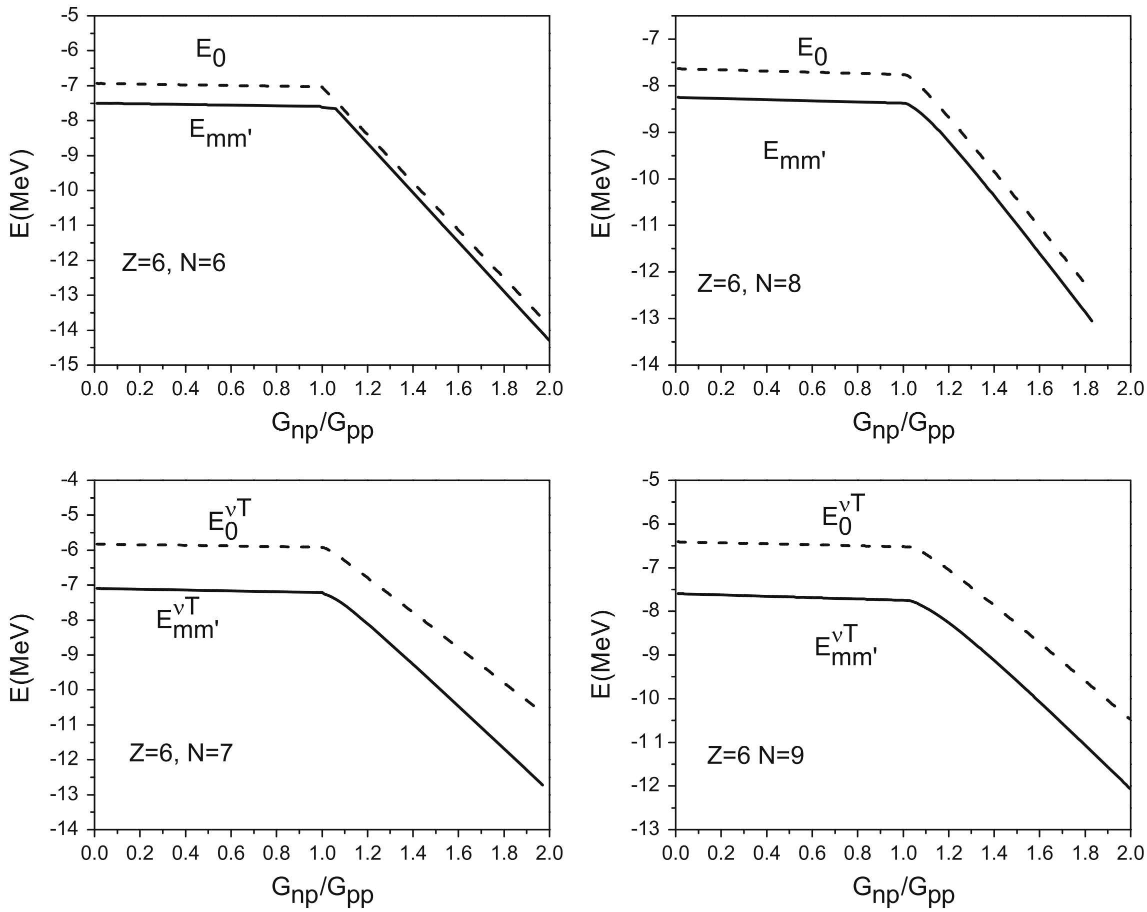

Fig. 3 Variation of the energy as a function of the ratio G_{np}/G_{pp}, within the one-level model using $\Omega = 12$ and $G_{nn} = G_{pp} = 0.125$ MeV, before (*dashed lines*) and after (*solid lines*) projection, for $Z = 6$ with $N - Z = 0, 1, 2, 3$

odd systems), the convergence is also rapidly reached in the case of the energy (as soon as $m = m' = 4$ in all the considered cases). However, the convergence seems to be slightly faster in even–even cases than in the odd ones.

As a second step, we have studied the variations of the energy, before [E_0, (respectively, $E_0^{\nu T}$)] and after ($E_{mm'}$, [respectively, $E_{mm'}^{\nu T}$)] the projection as a function of the ratio G_{np}/G_{pp}. The corresponding results are shown in Fig. 3 for $Z = 6$ (respectively, Fig. 4 for $Z = 8$) with $(N - Z) = 0, 1, 2, 3$. From these figures, one may conclude that the behavior of the energy as a function of G_{np} (before and after the projection) is similar in the even–even case and the odd one. Here again, there appears two regions, i.e. when $G_{np} < \left(G_{np}\right)_c$ and when $G_{np} > \left(G_{np}\right)_c$. The slope variation in the E_0 (respectively, $E_0^{\nu T}$) and $E_{mm'}$ (respectively, $E_{mm'}^{\nu T}$) curves corresponds to the value $G_{np} = \left(G_{np}\right)_c$. The fact that the energies are not constant when $G_{np} < \left(G_{np}\right)_c$, even if Δ_{nn} and Δ_{pp} are constant is due to the additional term in G_{np} in Eqs. (36), (38), (40) and (41).

Moreover, in every case, the projection effect leads to a lowering of the energy. One may also notice that the discrepancy between the BCS and projected energy values is constant for a given region. We reported in Table 9 (respectively, Table 10) the values of the relative discrepancy δE (%) between the projected and non-projected energies, as a function of $(N - Z)$, for $Z = 6$ and $Z = 8$ when $G_{np} = 0.75\, G_{pp}$ (respectively, when $G_{np} = 1.5\, G_{pp}$) to illustrate the region $G_{np} < \left(G_{np}\right)_c$ (respectively, $G_{np} > \left(G_{np}\right)_c$). It then appears that the projection effect is more important in the first region. It also appears that the projection effect is more important in odd systems than in the even–even ones. Indeed, the average value of δE is, respectively, 8 % when $G_{np} < \left(G_{np}\right)_c$ and 4% when $G_{np} > \left(G_{np}\right)_c$ in the even–even case, whereas it is 17 % when $G_{np} < \left(G_{np}\right)_c$ and 15 % when $G_{np} > \left(G_{np}\right)_c$ in the odd case. From the above, we can conclude on the necessity of the elimination of the false components in the BCS states in the odd-mass systems.

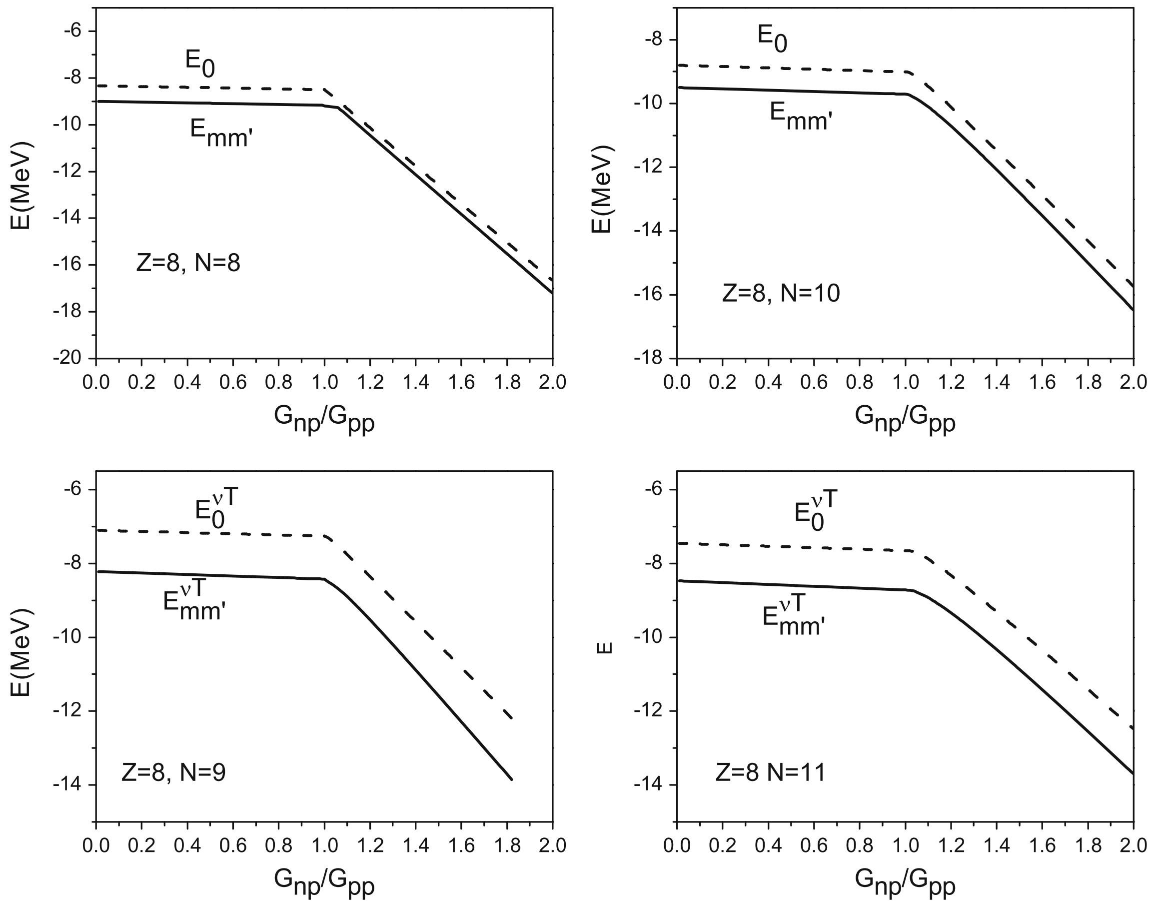

Fig. 4 Same as Fig. 3 for $Z = 8$ with $N - Z = 0, 1, 2, 3$

Table 9 Variation of the relative discrepancy δE (%) between the projected and non projected energies, as a function of $(N - Z)$, for $Z = 6$ (left part) and $Z = 8$ (right part) when $G_{np} = 0.75\ G_{pp}$

	$N - Z$	δE (%)		$N - Z$	δE (%)
$Z = 6$	0	8.03	$Z = 8$	0	7.89
	1	21.93		1	15.94
	2	7.94		2	7.79
	3	18.71		3	13.85

Table 10 Same as Table 9 when $G_{np} = 1.5\ G_{pp}$

	$N - Z$	δE (%)		$N - Z$	δE (%)
$Z = 6$	0	3.02	$Z = 8$	0	3.18
	1	19.09		1	13.58
	2	5.19		2	5.08
	3	15.71		3	10.58

Conclusion

A formalism that enables one to take into account the isovector pairing interaction, with inclusion of the particle-number conservation, in odd systems has been established. The Wahlborn blocking method has been used [44, 45].

The most general form of the isovector pairing Hamiltonian has been approximately diagonalized using the Wick theorem. A discrete expression of the projection operator has been constructed. A projection of the BCS wave function on both the good proton and neutron numbers has been performed. The expression of the ground-state projected energy has been deduced.

The method has been numerically tested using the one-level schematic model. The convergence of the method as a function of the extraction degrees of the false components has been studied. The rapidity of this convergence shows the efficiency of the projection method. On the other hand, it has been shown that the behavior of the energy as a function of the neutron–proton pairing constant in odd systems is analogous to that of even–even ones. However, this effect seems to be more important in odd systems.

Conflict of interest The authors declare that they have no competing interests.

Authors' contributions All authors, AB, MF, and ANH, contributed to the formalism. AB performed thenumerical calculations. All authors read and approved the final manuscript.

Appendix A

Limit when $\Delta_{np} \to 0$

Before projection

At the limit when $\Delta_{np} \to 0$, the coefficients B_i^j which appear in Eq. (10) become

$$\begin{array}{l} B_1^j = v_{jp}v_{jn}, \quad B_t^j = v_{jt}u_{jt'} \\ B_4^j = 0, \quad B_5^j = u_{jp}u_{jn} \end{array},$$

where $t = n, p$ and $t' \neq t$.

u_{vt} and v_{vt} are the occupation and inoccupation probability amplitudes of the v state in the conventional BCS theory (i.e. in the pairing between like-particles case).

It may be easily shown that the wave-function $|\Psi\rangle$ defined by (9) in the even–even case is then the product of the usual BCS wave-functions of the proton and neutron systems.

The energy of the system given by (14) reads in this case

$$\lim_{\Delta_{np}\to 0} E_0 = \sum_t \left[2\sum_{j>0} \varepsilon_{jt} v_{jt}^2 - G_{tt}\sum_{j>0} v_{jt}^4 - \frac{\Delta_{tt}^2}{G_{tt}} \right] - G_{np}\sum_{j>0} v_{jp}^2 v_{jn}^2 \tag{36}$$

This means that, in this case, E_0 is not only the sum of the energies of the proton and neutron systems, but also there is an additional term $\left(-G_{np}\sum_{j>0} v_{jp}^2 v_{jn}^2\right)$.

In the same way, the wave-function in the even–odd case defined by (11) becomes

$$\lim_{\Delta_{np}\to 0} |vT\rangle = a_{vT}^+ \prod_{\substack{t,j>0 \\ j\neq v}} \left(u_{jt} + v_{jt} a_{jt}^+ a_{\overline{jt}}^+ \right) |0\rangle \tag{37}$$

It is worth noticing that this expression does not exactly reduce to its homologue of the conventional BCS theory. Indeed, in the latter, the neutron and proton systems are considered separately. Thus, when a level of the t (say the proton) system is blocked, there is no consequence on the t' ($t' \neq t$) (the neutron) system. On the opposite, in the np pairing case, due to the definition of the wave function (11), the blocked level vT is simultaneously excluded for both types of nucleons (i.e. the protons and the neutrons).

As for the expression of the energy given by (17), it becomes

$$\lim_{\Delta_{np}\to 0} E_0^{vT} = \varepsilon_{vT} + \sum_t \left[2\sum_{\substack{j>0 \\ j\neq v}} \varepsilon_{jt} v_{jt}^2 - G_{tt}\sum_{\substack{j>0 \\ j\neq v}} v_{jt}^4 - \frac{\left(\Delta_{tt}^{(v)}\right)^2}{G_{tt}} \right] - G_{np}\sum_{\substack{j>0 \\ j\neq v}} v_{jp}^2 v_{jn}^2 \tag{38}$$

As in the even–even case, the term $\left(-G_{np}\sum_{\substack{j>0 \\ j\neq v}} v_{jp}^2 v_{jn}^2\right)$ appears in addition to the sum of the proton and neutron system energies.

After projection

As it was the case before projection, one may easily verify that in the even–even case, $|\Psi_{mm'}\rangle$ reduces to the product of the projected wave-functions of the neutron and proton systems in the pairing between like-particles case defined in Reference [41].

The corresponding energy is given by

$$\lim_{\Delta_{np}\to 0} E_{mm'} = E_m + E_{m'} - 4G_{np}(m+1)(m'+1)C_m^2 C_{m'}^2 \times \left\{ \sum_{k=0}^{m+1}\sum_{k'=0}^{m'+1} \xi_k \xi_{k'} \left[z_k^{-P_N+1} z_{k'}^{-P_Z+1} \sum_{j>0} v_{jn}^2 v_{jp}^2 \prod_{i\neq j} (u_{in}^2 + z_k v_{in}^2)(u_{ip}^2 + z_{k'} v_{ip}^2) + \overline{z}_k^{-P_N+1} z_{k'}^{-P_Z+1} \sum_{j>0} v_{jn}^2 v_{jp}^2 \prod_{i\neq j} (u_{in}^2 + \overline{z}_k v_{in}^2) \times \left(u_{ip}^2 + z_{k'} v_{ip}^2 \right) \right] + c.c \right\} \tag{39}$$

where E_m is the projected energy of the neutron system and $E_{m'}$ that of the proton system in the pairing between like-particles case for an even system and C_m and $C_{m'}$ are the corresponding normalization constants (see Reference [41]). This means that at the limit when $\Delta_{np} \to 0$, the energy (31) does not only reduces to the sum of the proton and neutron systems energies.

In the even–odd case, the wave function $|vT_{mm'}\rangle$ defined by Eq. (26) becomes

$$\lim_{\Delta_{np}\to 0} |vT_{mm'}\rangle = a_{vT}^+ C_{mv} \left\{ \sum_{k=0}^{m+1} \xi_k \left[z_k^{-P_N} \prod_{\substack{j>0 \\ j\neq v}} \left(u_{jn} + z_k v_{jn} A_{jn}^+ + \right) |0\rangle + cc \right] \right\} \times C_{m'v} \left\{ \sum_{k'=0}^{m'+1} \xi_{k'} \left[z_{k'}^{-P_Z} \prod_{\substack{j>0 \\ j\neq v}} \left(u_{jp} + z_{k'} v_{jp} A_{jp}^+ \right) |0\rangle + cc \right] \right\} \tag{40}$$

C_{mv} and $C_{m'v}$ being the normalization constants.

As it was already the case before the projection, this expression does not exactly generalizes that of the pairing between like-particles case. Indeed, the blocked level is excluded from the products in both systems. In the same way, the energy (35) reads

$$\lim_{\Delta_{np}\to 0} E^{\nu T}_{mm'} = \varepsilon_{\nu T} + E^{\nu}_{m} + E^{\nu}_{m'} - 4G_{np}(m+1)(m'+1)C^2_{m\nu}C^2_{m'\nu}\left\{\sum_{k=0}^{m+1}\sum_{k'=0}^{m'+1}\xi_k\xi_{k'} \times \left[z_k^{-P_N+1} z_{k'}^{-P_Z+1}\sum_{j\neq\nu} v^2_{jn}v^2_{jp}\prod_{i\neq j\neq\nu}(u^2_{in}+z_k v^2_{in})(u^2_{ip}+z_{k'}v^2_{ip}) + \bar{z}_k^{-P_N+1} z_{k'}^{-P_Z+1}\sum_{j\neq\nu} v^2_{jn}v^2_{jp}\prod_{i\neq j\neq\nu}(u^2_{in}+\bar{z}_k v^2_{in})(u^2_{ip}+z_{k'}v^2_{ip})\right] + c.c\right\} \tag{41}$$

where

$$E^{\nu}_{m} = 2(m+1)C^2_{m\nu}\left\{\sum_{k=0}^{m+1}\xi_k z_k^{-P+1} \times \left[\sum_{j\neq\nu} 2\left(\varepsilon_j - \frac{G}{2}\right)v_j^2 \prod_{i\neq j\neq\nu}(u_i^2+z_k v_i^2) - 2G\sum_{\substack{l<i\\ l\neq\nu}} u_j v_j u_l v_l \prod_{i\neq\nu,j,l}(u_i^2+z_k v_i^2)\right] + cc\right\} \tag{42}$$

One notices that although $\Delta_{np}\to 0$, there remains a term in G_{np}. Moreover, as before the projection, the blocked level concerns both the proton and neutron systems.

Appendix B

Extraction of the real parts

Normalization constants

The real part of Eq. (29) is given by:

$$C^{-2}_{mm'} = 8(m+1)(m'+1)\sum_{k=0}^{m+1}\sum_{k'=0}^{m'+1}\xi_k\xi_{k'} \times \left[\rho(x_k,x_{k'})\cos\theta(x_k,x_{k'}) + \rho(-x_k,x_{k'}) \times \cos\theta(-x_k,x_{k'})\right] \tag{43}$$

with

$$x_k = \frac{k\pi}{2(m+1)}$$

$$\theta(x_k,x_{k'}) = -2P_N x_k - 2P_Z x_{k'} + \varphi(x_k,x_{k'})$$

$$\rho(x_k,x_{k'}) = \prod_{j>0}\rho_j(x_k,x_{k'}), \quad \varphi(x_k,x_{k'}) = \sum_{j>0}\varphi_j(x_k,x_{k'})$$

$$\rho_j(x_k,x_{k'}) = \sqrt{(a^{(j)})^2+(b^{(j)})^2}, \quad \tan\varphi_j(x_k,x_{k'}) = \frac{b^{(j)}}{a^{(j)}}$$

where

$$a^{(j)} = (B_1^j)^2\cos(2x_k+2x_{k'}) + (B_p^j)^2\cos 2x_{k'} + (B_n^j)^2\cos 2x_k + 2(B_4^j)^2\cos(x_k+x_{k'}) + (B_5^j)^2$$

$$b^{(j)} = (B_1^j)^2\sin(2x_k+2x_{k'}) + (B_p^j)^2\sin 2x_{k'} + (B_n^j)^2\sin 2x_k + 2(B_4^j)^2\sin(x_k+x_{k'})$$

In the same way, the real part of Eq. (34) reads

$$C^{-2}_{\nu mm'} = 8(m+1)(m'+1)\sum_{k=0}^{m+1}\sum_{k'=0}^{m'+1}\xi_k\xi_{k'} \times \left[\frac{\rho(x_k,x_{k'})}{\rho_\nu(x_k,x_{k'})}\cos\theta_\nu(x_k,x_{k'}) + \frac{\rho(-x_k,x_{k'})}{\rho_\nu(-x_k,x_{k'})}\cos\theta_\nu(-x_k,x_{k'})\right] \tag{44}$$

where

$$\theta_{i\ldots j}(x_k,x_{k'}) = \theta(x_k,x_{k'}) - \varphi_i(x_k,x_{k'}) - \ldots - \varphi_j(x_k,x_{k'})$$

Energy

The real part of the energy for an even–even system [Eq. (31)] is given by

$$E_{mm'} = 8(m+1)(m'+1)C^2_{mm'}\sum_{k=0}^{m+1}\sum_{k'=0}^{m'+1}\xi_k\xi_{k'} \times \left\{\sum\left[\varepsilon_j(x_k,x_{k'}) + \varepsilon_j(-x_k,x_{k'})\right] + \sum_{\substack{j,l>0\\ j\neq l}}\left[\varepsilon_{jl}(x_k,x_{k'}) + \varepsilon_{jl}(-x_k,x_{k'})\right]\right\}, \tag{45}$$

where

$$\varepsilon_j(x_k,x_{k'}) = \frac{\rho(x_k,x_{k'})}{\rho_j(x_k,x_{k'})}\{R_0^j(x_k,x_{k'})\cos\Phi_0^j(x_k,x_{k'}) - G_{nn}R_n^j(x_{k'})\cos\Phi_n^j(x_k,x_{k'}) - G_{pp}R_p^j(x_k)\cos\Phi_p^j(x_k,x_{k'}) - G_{np}R_{np}^j(x_k,x_{k'})\cos\Phi_{np}^j(x_k,x_{k'})\} \tag{46}$$

and

$$\varepsilon_{jl}(x_k,x_{k'}) = \frac{\rho(x_k,x_{k'})}{\rho_j(x_k,x_{k'})\rho_l(x_k,x_{k'})} \times \{-G_{nn}Q_n^j(x_{k'})Q_n^l(x_{k'})\cos\Phi_n^{jl}(x_k,x_{k'}) - G_{pp}Q_p^j(x_k)Q_p^l(x_k)\cos\Phi_p^{jl}(x_k,x_{k'}) - 2G_{np}Q_{np}^j(x_k,x_{k'})Q_{np}^l(x_k,x_{k'})\cos\Phi_{np}^{jl}(x_k,x_{k'})\} \tag{47}$$

with the notations

$$\begin{aligned}
R_0^j(x_k,x_{k'}) &= \sqrt{(a_0^{(j)})^2 + (b_0^{(j)})^2}\\
\eta_0^j(x_k,x_{k'}) &= \arctan\left(\frac{b_0^{(j)}}{a_0^{(j)}}\right)\\
R_i^j(x_k,x_{k'}) &= \sqrt{(a_{i1}^{(j)})^2 + (b_{i1}^{(j)})^2}\\
\eta_i^j(x_k,x_{k'}) &= \arctan\left(\frac{b_{i1}^{(j)}}{a_{i1}^{(j)}}\right)\\
Q_i^j(x_k,x_{k'}) &= \sqrt{(a_{i2}^{(j)})^2 + (b_{i2}^{(j)})^2}\\
\delta_i^j(x_k,x_{k'}) &= \arctan\left(\frac{b_{i2}^{(j)}}{a_{i2}^{(j)}}\right)\\
i &= n\,,\ p\,,\ np
\end{aligned} \tag{48}$$

$$\begin{aligned}
\Phi_0^j(x_k,x_{k'}) &= \theta_j(x_k,x_{k'}) + \eta_0^j(x_k,x_{k'})\\
\Phi_n^j(x_k,x_{k'}) &= \theta_j(x_k,x_{k'}) + \eta_n^j(x_{k'}) + 2x_k\\
\Phi_p^j(x_k,x_{k'}) &= \theta_j(x_k,x_{k'}) + \eta_p^j(x_k) + 2x_{k'}\\
\Phi_{np}^j(x_k,x_{k'}) &= \theta_j(x_k,x_{k'}) + \eta_{np}^j(x_k,x_{k'})\\
\Phi_n^{jl}(x_k,x_{k'}) &= \theta_{jl}(x_k,x_{k'}) + \delta_n^j(x_{k'}) + \delta_n^l(x_{k'}) + 2x_k\\
\Phi_p^{jl}(x_k,x_{k'}) &= \theta_{jl}(x_k,x_{k'}) + \delta_p^j(x_k) + \delta_p^l(x_k) + 2x_{k'}\\
\Phi_{np}^{jl}(x_k,x_{k'}) &= \theta_{jl}(x_k,x_{k'}) + \delta_{np}^j(x_k,x_{k'}) + \delta_{np}^l(x_k,x_{k'}) + x_k + x_{k'}
\end{aligned} \tag{49}$$

$$\begin{aligned}
\theta(x_k,x_{k'}) &= -2P_N x_k - 2P_Z x_{k'} + \varphi(x_k,x_{k'})\\
\theta_{iqr}(x_k,x_{k'}) &= \theta_i(x_k,x_{k'}) + qx_k + rx_{k'}\\
\theta_{i\ldots jqr}(x_k,x_{k'}) &= \theta_{i\ldots j}(x_k,x_{k'}) + qx_k + rx_{k'}
\end{aligned} \tag{50}$$

$$\begin{aligned}
a_0^{(j)} &= 2(B_1^j)^2(\varepsilon_{jn}+\varepsilon_{jp})\cos(2x_k+2x_{k'}) + 2(B_p^j)^2\varepsilon_{jp}\cos 2x_{k'} + 2(B_n^j)^2\varepsilon_{jn}\cos 2x_k + 2(B_4^j)^2(\varepsilon_{jn}+\varepsilon_{jp})\cos(x_k+x_{k'})\\
b_0^{(j)} &= 2(B_1^j)^2(\varepsilon_{jn}+\varepsilon_{jp})\sin(2x_k+2x_{k'}) + 2(B_p^j)^2\varepsilon_{jp}\sin 2x_{k'} + 2(B_n^j)^2\varepsilon_{jn}\sin 2x_k + 2(B_4^j)^2(\varepsilon_{jn}+\varepsilon_{jp})\sin(x_k+x_{k'})
\end{aligned} \tag{51}$$

$$\begin{aligned}
a_{n1}^{(j)} &= (B_1^j)^2\cos 2x_{k'} + (B_n^j)^2; \quad b_{n1}^{(j)} = (B_1^j)^2\sin 2x_{k'}\\
a_{p1}^{(j)} &= (B_1^j)^2\cos 2x_k + (B_p^j)^2; \quad b_{p1}^{(j)} = (B_1^j)^2\sin 2x_k
\end{aligned} \tag{52}$$

$$\begin{aligned}
a_{np1}^{(j)} &= (B_1^j)^2\cos(2x_k+2x_{k'}) + 2(B_4^j)^2\cos(x_k+x_{k'})\\
b_{np1}^{(j)} &= (B_1^j)^2\sin(2x_k+2x_{k'}) + 2(B_4^j)^2\sin(x_k+x_{k'})
\end{aligned} \tag{53}$$

$$\begin{aligned}
a_{n2}^{(j)} &= B_1^jB_p^j\cos 2x_{k'} + B_n^jB_5^j; \quad b_{n2}^{(j)} = B_1^jB_p^j\sin 2x_{k'}\\
a_{p2}^{(j)} &= B_1^jB_n^j\cos 2x_k + B_p^jB_5^j; \quad b_{p2}^{(j)} = B_1^jB_n^j\sin 2x_k
\end{aligned} \tag{54}$$

$$\begin{aligned}
a_{np2}^{(j)} &= B_1^jB_4^j\cos(x_k+x_{k'}) - B_4^jB_5^j\\
b_{np2}^{(j)} &= B_1^jB_4^j\sin(x_k+x_{k'})
\end{aligned} \tag{55}$$

In the same way, for an even–odd system, the real part of the energy (Eq. (35)) is given by

$$E_{mm'}^{\nu T} = \varepsilon_{\nu T} + 8(m+1)(m'+1)C_{\nu mm'}^2 \times \sum_{k=0}^{m+1}\sum_{k'=0}^{m'+1}\xi_k\xi_{k'}\left\{\sum_{\substack{j>0\\ j\neq\nu}}\left[\varepsilon_j^\nu(x_k,x_{k'}) + \varepsilon_j^\nu(-x_k,x_{k'})\right] + \sum_{\substack{j,l>0\\ j\neq l\\ j\neq\nu}}\left[\varepsilon_{jl}^\nu(x_k,x_{k'}) + \varepsilon_{jl}^\nu(-x_k,x_{k'})\right]\right\} \tag{56}$$

where

$$\varepsilon_j^\nu(x_k,x_{k'}) = \frac{\rho(x_k,x_{k'})}{\rho_j(x_k,x_{k'})\rho_\nu(x_k,x_{k'})} \times \{R_0^j(x_k,x_{k'})\cos\Phi_0^{j\nu}(x_k,x_{k'}) - G_{nn}R_n^j(x_{k'})\cos\Phi_n^{j\nu}(x_k,x_{k'}) - G_{pp}R_p^j(x_k)\cos\Phi_p^{j\nu}(x_k,x_{k'}) - G_{np}R_{np}^j(x_k,x_{k'})\cos\Phi_{np}^{j\nu}(x_k,x_{k'})\} \tag{57}$$

and

$$\varepsilon_{jl}^\nu(x_k,x_{k'}) = \frac{\rho(x_k,x_{k'})}{\rho_j(x_k,x_{k'})\rho_l(x_k,x_{k'})\rho_\nu(x_k,x_{k'})} \{-G_{nn}Q_n^j(x_{k'})Q_n^l(x_{k'})\cos\Phi_n^{jl\nu}(x_k,x_{k'}) - G_{pp}Q_p^j(x_k)Q_p^l(x_k)\cos\Phi_p^{jl\nu}(x_k,x_{k'}) - 2G_{np}Q_{np}^j(x_k,x_{k'})Q_{np}^l(x_k,x_{k'})\cos\Phi_{np}^{jl\nu}(x_k,x_{k'})\} \tag{58}$$

with the notations

$$\begin{aligned}
\Phi_0^{j\nu}(x_k,x_{k'}) &= \theta_{j\nu}(x_k,x_{k'}) + \eta_0^j(x_k,x_{k'})\\
\Phi_n^{j\nu}(x_k,x_{k'}) &= \theta_{j\nu}(x_k,x_{k'}) + \eta_n^j(x_{k'}) + 2x_k\\
\Phi_p^{j\nu}(x_k,x_{k'}) &= \theta_{j\nu}(x_k,x_{k'}) + \eta_p^j(x_k) + 2x_{k'}\\
\Phi_{np}^{j\nu}(x_k,x_{k'}) &= \theta_{j\nu}(x_k,x_{k'}) + \eta_{np}^j(x_k,x_{k'})\\
\Phi_n^{jl\nu}(x_k,x_{k'}) &= \theta_{jl\nu}(x_k,x_{k'}) + \delta_n^j(x_{k'}) + \delta_n^l(x_{k'}) + 2x_k\\
\Phi_p^{jl\nu}(x_k,x_{k'}) &= \theta_{jl\nu}(x_k,x_{k'}) + \delta_p^j(x_k) + \delta_p^l(x_k) + 2x_{k'}\\
\Phi_{np}^{jl\nu}(x_k,x_{k'}) &= \theta_{jl\nu}(x_k,x_{k'}) + \delta_{np}^j(x_k,x_{k'}) + \delta_{np}^l(x_k,x_{k'}) + x_k + x_{k'}
\end{aligned} \tag{59}$$

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