Correcting for self-pairing and poles in the PNP-HFB method

I. Formal aspects

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Outlook

I. HFB and PNP-HFB methods

II. Divergences and poles in the PNP-HFB method

III. Physical interpretation of the problem

IV. Formal solution to it

V. Application in one realistic case

VI. Conclusions: more advanced problems to be solved
Pairing

I. Impact of pairing correlations on nuclear structure/neutron stars properties

*Individual excitation spectra
*Odd-even mass staggering
*Rotational and low-lying vibrational states as well as shape isomers
*Width of deep-hole states
*Matter density
*Pair transfer
*Glitches in the inner crust of neutron stars
*Cooling of neutron stars: emission processes and heat diffusion

II. Methods for realistic calculations of finite nuclei

*Symmetry conserving: HF + shell-model + quadrupole correlations  Volya et al. (2001)

Pillet et al. (2002)

*Symmetry breaking: HFB + PNP + Pairing vib. + def. and coupl. to surf/vol vib.

III. PNP-HFB/HFBCS calculations with DD forces within the full s.p. space

*GCM+PAV with Skyrme + DDDI pairing  Heenen et al. (1993)

*PAV/VAP with Gogny  Anguiano et al. (2001)
Realistic PNP-HFB calculations of nuclear properties

I. Abilities beyond HFB

* Restore a good quantum number
* VAP/constr. calc. + PAV - good treatment of correlations in the weak symmetry breaking regime
* VAP: correlations in the wave-function near closed shells (other observables than energies)
* PNP practical when coupled to GCM
* PNP + Pairing vibrations: additional correlations + excited states

II. Canonical basis of the HFB state

HFB

\[ |\Phi(\varphi)\rangle = \prod_{\mu > 0} (u_\mu + v_\mu e^{2i\varphi} a_\mu^\dagger a_\mu^\dagger) |0\rangle \]

Observable are independent of \( \varphi \):

\[ E = \frac{\langle \Phi(0)|H|\Phi(0)\rangle}{\langle \Phi(0)|\Phi(0)\rangle} \]

PNP-HFB

\[ |\Psi^N\rangle = \hat{P}^N |\Phi(0)\rangle = \frac{1}{2\pi} \int_0^{2\pi} d\varphi e^{-i\varphi N} |\Phi(\varphi)\rangle \]

Diagonal density matrix and pairing tensor:

\[ \rho_{\varphi \mu \mu} = \rho_{0 \mu \mu} = v_\mu^2 \]

\[ \kappa_{\varphi \mu \bar{\mu}} = \kappa_{0 \mu \bar{\mu}} = u_\mu v_{\bar{\mu}} \]

\[ \kappa_{\varphi \mu \bar{\mu}}^* = \kappa_{0 \mu \bar{\mu}}^* = u_\mu v_{\bar{\mu}} \]

Transition density matrix and pairing tensor:

\[ \rho_{\mu \mu}(\varphi) = v_\mu^2 e^{2i\varphi} / (u_\mu^2 + v_\mu^2 e^{2i\varphi}) \]

\[ \kappa_{\mu \mu}^{10}(\varphi) = u_\mu v_{\bar{\mu}} e^{2i\varphi} / (u_\mu^2 + v_\mu^2 e^{2i\varphi}) \]

\[ \kappa_{\mu \mu}^{01}(\varphi) = u_\mu v_{\bar{\mu}} / (u_\mu^2 + v_\mu^2 e^{2i\varphi}) \]

\[ E^N = \frac{\langle \Phi(0)|H\hat{P}^N|\Phi(0)\rangle}{\langle \Phi(0)|\hat{P}^N|\Phi(0)\rangle} \]
Problem with PNP-HFB method I

PES: $^{18}O$

3D PNP-HFBLN (PAV)

SLy4 + ULB

9 $\varphi$-integration points

*Typical of calculations performed so far

*Results look very reasonable
Problem with PNP-HFB method II

**PES:** $^{18}O$

3D PNP-HFBLN (PAV)

SLy4+ULB

9/99 $\varphi$-integration points

*Divergence when a pair of states crosses $\lambda$, Anguiano et al. (2001)*

*Offset in the PES before and after the crossing, Dobaczewski et al. priv. comm.*

*More dramatic consequences for VAP calculations*
What are HFB and PNP-HFB really about?

I. HFB: energy functional of $\rho$ and $\kappa$ (bilinear here)

$$
\mathcal{E} [\rho, \kappa, \kappa^*] = \sum_{ij} t_{ij} \rho_{ji} + \sum_{ijkl} \left[ w_{ijkl}^{\rho\rho} \rho_{ji} \rho_{lk} + w_{ikjl}^{\kappa\kappa} \kappa_{ik} \kappa_{jl} \right] \neq \frac{\langle \Phi(\varphi)|H|\Phi(\varphi)\rangle}{\langle \Phi(\varphi)|\Phi(\varphi)\rangle}
$$

II. PNP-HFB: $\mathcal{E}^N$ is real and independent of the choice of axis in gauge space

$$
\mathcal{E}^N = \frac{\int_{0}^{2\pi} d\varphi \ e^{-i\varphi N} \mathcal{E} [\varphi] \ I(\varphi)}{\int_{0}^{2\pi} d\varphi \ e^{-i\varphi N} I(\varphi)} \quad \text{with} \quad I(\varphi) = \langle \Phi(0)|\Phi(\varphi)\rangle = \prod_{\nu > 0} (u^2_\nu + v^2_\nu e^{2i\varphi})
$$

$*$\mathcal{E} [\varphi] \equiv "\langle \Phi(0)|H|\Phi(\varphi)\rangle" \rightarrow \mathcal{E} [\rho, \kappa, \kappa^*]$ for $\varphi \rightarrow 0$

$*$\mathcal{E} [\varphi]$ might depend on $[\rho_0, \kappa_0, \kappa_0^*], [\rho_\varphi, \kappa_\varphi, \kappa_\varphi^*], [\rho(\varphi), \kappa^{10}(\varphi), \kappa^{01}(\varphi)]$

$*$No fully satisfactory constructive framework exists so far
### III. Motivations

<table>
<thead>
<tr>
<th>HFB</th>
<th>PNP-HFB</th>
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<tbody>
<tr>
<td>$\mathcal{E} [\rho, \kappa, \kappa^*]$</td>
<td>$\mathcal{E} [\varphi]$</td>
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\[
\langle \Phi(0)|V^{(2)}|\Phi(\varphi)\rangle \text{ (GWT)} \quad \rho \rho / \kappa^* \kappa \quad \rightarrow \quad \rho(\varphi) \rho(\varphi) / \kappa^{01}(\varphi) \kappa^{10}(\varphi)
\]

\[
\langle \Phi(0)|V^{(3)}|\Phi(\varphi)\rangle \text{ (GWT)} \quad \rho \rho \rho / \kappa^* \kappa \rho \quad \rightarrow \quad \rho(\varphi) \rho(\varphi) \rho(\varphi) / \kappa^{01}(\varphi) \kappa^{10}(\varphi) \rho(\varphi)
\]

2-body correl. (MBPT) \quad $\rho \rho \rho^\alpha$ \quad $\rightarrow$ \quad $\rho(\varphi) \rho(\varphi) \rho_0^\alpha$ \quad T. D. (2004)

Pairing regularization \quad $\kappa^* \kappa \rho^\gamma$ \quad $\rightarrow$ \quad $\kappa^{01}(\varphi) \kappa^{10}(\varphi) \rho_0^\gamma$ \quad T. D. (unpublished)

Coulomb Exchange (Slater) \quad $\rho_p \rho_p^{1/3}$ \quad $\rightarrow$ \quad $?$

### IV. Bilinear functional "from $V^{(2)}"$

\[
\mathcal{E}^N = \int_0^{2\pi} d\varphi \frac{e^{-i\varphi N}}{2\pi D_N} \left[ \sum_{\mu} t_{\mu\mu} \rho_{\mu\mu}(\varphi) + \sum_{\mu\nu} w^{\rho\rho}_{\mu\nu\mu\nu} \rho_{\mu\mu}(\varphi) \rho_{\nu\nu}(\varphi) + \sum_{\mu\nu} w^{\kappa\kappa}_{\mu\nu\mu\nu} \kappa^{01}_{\mu\mu}(\varphi) \kappa^{10}_{\nu\nu}(\varphi) \right] \prod_{\nu > 0} (u_{\nu}^2 + v_{\nu}^2 e^{2i\varphi})
\]

*Potential divergences from terms such that $\nu = \mu, \bar{\mu}$
*Cancel out if $\bar{w}^{\rho\rho}_{\mu\nu\mu\nu} = \bar{w}^{\kappa\kappa}_{\mu\nu\mu\nu}$
*The problem is "conjugated pair additive"
Complex plane analysis

*Dobaczewski et al. unpublished*

\[ Z = |Z| \text{Exp}(i \phi) \]

\[ \mathcal{E}[Z] \]

Poles: \( Z_k = \pm i |u_k|/|v_k| \)

Integration circle: \(|r| = 1\)

\[ z = e^{i \phi} \]

\(*\mathcal{E}^N: \) poles at \( z_{\mu}^\pm = \pm i |u_{\mu}|/|v_{\bar{\mu}}| \) and \( z = 0 \)

\(*\text{Cauchy: } |z| < 1 \) contribute to \( \mathcal{E}^N \)

\(*\text{Only } z = 0 \) contributes for \( H \)

\(*\text{Divergence in } \mathcal{E}^N \) when poles cross \( C_1 \)

\(*\text{Step left in } \mathcal{E}^N \) after the crossing

\(*\text{Is that physical?} \)

\(*\text{Is there a solution to those problems?} \)
I. HFB

*Self-interaction issue \( \mathcal{E}_\mu = t_{\mu\mu} v_\mu^2 + w_{\mu\mu\mu\mu}^\rho v_\mu^4 \neq t_{\mu\mu} \rho_{\mu\mu} \)

*Self-pairing issue

\[
\mathcal{E}_{\mu\bar{\mu}} - (\mathcal{E}_\mu + \mathcal{E}_{\bar{\mu}}) = \left( w_{\mu\bar{\mu}\mu\bar{\mu}}^{\rho\rho} + w_{\mu\mu\bar{\mu}\bar{\mu}}^{\rho\rho} \right) v_\mu^4 + 4 w_{\mu\bar{\mu}\mu\bar{\mu}}^{\kappa\kappa} u_{\mu}^2 v_\mu^2 \neq \bar{w}_{\mu\bar{\mu}\mu\bar{\mu}}^{\rho\rho} \rho_{\mu\bar{\mu}\mu\bar{\mu}}^{(2)} 
\]

where \( \rho_{\mu\bar{\mu}\mu\bar{\mu}}^{(2)} = \frac{\langle \Phi(\varphi) | a_\mu^\dagger a_{\bar{\mu}}^\dagger a_{\bar{\mu}} a_\mu | \Phi(\varphi) \rangle}{\langle \Phi(\varphi) | \Phi(\varphi) \rangle} = v_\mu^2 \)

*Spurious contributions to the energy

*Pair additive problem

*Self-interaction is well known in Kohn-Sham DFT, Perdew and Zunger (1981)

*None of the two has been explored in nuclear structure calculations so far
II. PNP-HFB

*Self-interaction issue

\[
\mathcal{E}^N_{\mu} = \int_0^{2\pi} d\phi \frac{e^{-i\phi N}}{2\pi D_N} \left[ t_{\mu\mu} + w^{\rho\rho}_{\mu\mu\mu\mu} \frac{v^2_{\mu} e^{2i\phi}}{u^2_{\mu} + v^2_{\mu} e^{2i\phi}} \right] v^2_{\mu} e^{2i\phi} \prod_{\nu \neq \mu > 0} (u^2_{\nu} + v^2_{\nu} e^{2i\phi}) \neq t_{\mu\mu} \rho_{\mu\mu}^N
\]

*Self-pairing issue

\[
\mathcal{E}^N_{\mu\mu} - (\mathcal{E}^N_{\mu} + \mathcal{E}^N_{\mu}) = \int_0^{2\pi} d\phi \frac{e^{-i\phi N}}{2\pi D_N} \left[ (w^{\rho\rho}_{\mu\mu\mu\mu} + w^{\rho\rho}_{\mu\mu\mu\mu}) v^2_{\mu} e^{2i\phi} + 4 w^{\kappa\kappa}_{\mu\mu\mu\mu} u^2_{\mu} \right] \frac{v^2_{\mu} e^{2i\phi}}{u^2_{\mu} + v^2_{\mu} e^{2i\phi}} \prod_{\nu \neq \mu > 0} (u^2_{\nu} + v^2_{\nu} e^{2i\phi}) \neq \bar{w}^{\rho\rho}_{\mu\mu\mu\mu} \rho_{\mu\mu\mu\mu}^N
\]

where

\[
\rho_{\mu\mu\mu\mu}^N(2) = \frac{\langle \Psi^N | a_{\mu}^\dagger a_{\mu}^\dagger a_{\mu} a_{\mu} | \Psi^N \rangle}{\langle \Psi^N | \Psi^N \rangle} = v^2_{\mu} \int_0^{2\pi} d\phi \frac{e^{-i\phi N}}{2\pi D_N} e^{2i\phi} \prod_{\nu \neq \mu > 0} (u^2_{\nu} + v^2_{\nu} e^{2i\phi}) = \rho_{\mu\mu}^N
\]

*Pair additive problem

*More dramatic than at the mean-field level
A minimal solution to the problem: motivation from $H$

*Pair additive problem $\implies$ Toy model with only one pair rotated: \[
\left(\begin{array}{c}
u \
\varphi
\end{array}\right) = \left(\begin{array}{c}1 \\ 0 \\
\exp(2i\varphi)
\end{array}\right)
\]

\[
|\phi(\varphi)\rangle = (u + v\exp(2i\varphi) a\dagger a\dagger) \prod_{\nu\neq\mu>0} (u + v\exp(2i\varphi) a\dagger a\dagger)|0\rangle = e^{i\varphi} \cos \varphi |\phi(0)\rangle - ie^{i\varphi} \sin \varphi |\phi(\frac{\pi}{2})\rangle
\]

*Using the Standard Wick Theorem (SWT)

\[
\mathcal{E}_{R/R}(\varphi)_{SWT} = e^{i\varphi} \cos \varphi \mathcal{E}_{R/R}(0)_{SWT} - ie^{i\varphi} \sin \varphi \mathcal{E}_{R/R}(\frac{\pi}{2})_{SWT}
\]

*Using the GWT

\[
\mathcal{E}_{R/R}(\varphi)_{GWT} = \mathcal{E}_{R/R}(\varphi)_{SWT} + \left( w_{R/R/R/R}^{R/R} + w_{R/R/R/R}^{R/R} + w_{R/R/R/R}^{R/R} + w_{R/R/R/R}^{R/R} \right) u^2 v^2 \frac{e^{2i\varphi} (e^{2i\varphi} - 1)}{u^2 + v^2 e^{2i\varphi}}
\]

\[
\mathcal{E}_{K/K}(\varphi)_{GWT} = \mathcal{E}_{K/K}(\varphi)_{SWT} - 4 w_{K/K/R/R}^{K/K} u^2 v^2 \frac{e^{2i\varphi} (e^{2i\varphi} - 1)}{u^2 + v^2 e^{2i\varphi}}
\]

*Spurious terms are directly related to the use of the GWT at finite $\varphi$

*Identification of the spurious terms to be removed

*Doing so does not change the HFB functional ($= \text{functional at } \varphi = 0$)

*Correct dramatic self-interaction/-pairing effects at the PNP-HFB level but not at the HFB level
Spurious contribution to $E^N$ in realistic PNP-HFB

I. Integration in real space

$$E^N_{spu.} = \sum_{\mu>0} \left[ (w_{\mu} + w_{\mu}^{\overline{\mu}} + w_{\mu}^{\overline{\mu}} + w_{\mu}^{\overline{\mu}}) - 4 w_{\mu}^{\overline{\mu}} \right] u_{\mu}^2 v_{\overline{\mu}}^4 \int_{0}^{2\pi} d\varphi \frac{e^{-i\varphi} e^{2i\varphi} - 1}{2i N} \frac{e^{2i\varphi}}{(u_{\mu}^2 + v_{\overline{\mu}}^2 e^{2i\varphi})^2} \prod_{\nu>0} (u_{\nu}^2 + v_{\overline{\nu}}^2 e^{2i\varphi})$$

II. Integration in the complex plane

*Pole at $0 < |z_{\mu}^-| < 1 \implies$ remove completely the contribution of the pole to $E^N$

$$Re_{spu.}(z_{\mu}^\pm) = -\left( \frac{v_{\mu}}{u_{\mu}} \right)^N \frac{1 + (-1)^N}{2i N} \prod_{\nu \neq \mu > 0} \frac{u_{\nu}^2 v_{\overline{\nu}}^2 - v_{\nu}^2 u_{\overline{\mu}}^2}{v_{\overline{\mu}}^2}$$

*Pole at $z = 0$ of order $N - 1 \iff$ more than just removing the spurious poles!

$$Re_{spu.}^2(0)_{\mu} = -\frac{1}{u_{\mu}^2} \prod_{\nu \neq \mu > 0} u_{\nu}^2$$

$$Re_{spu.}^N(0)_{\mu} = -\frac{v_{\mu}^2}{u_{\mu}^2} Re_{spu.}^{N-2}(0)_{\mu} + \frac{1}{u_{\mu}^2} \left[ \sum_{\{\lambda\}_{n-2}} \prod_{\nu \neq \mu,\{\lambda\}} u_{\nu}^2 \prod_{\{\lambda\}} v_{\lambda}^2 - \sum_{\{\lambda\}_{n-1}} \prod_{\nu \neq \mu,\{\lambda\}} u_{\nu}^2 \prod_{\{\lambda\}} v_{\lambda}^2 \right]$$
Conclusions and perspectives

I. PNP-HFB/PAV calculations

* Complete solution to the problem of divergences and jumps
* Solution exists for any type of higher-order density dependences
* Quantitative calculations: order of magnitude, stability, impact (see next)

II. PNP-HFB/VAP calculations

* The correction to $\mathcal{E}^N$ is precise and stable enough to be applied to VAP calculations
* Corrections to the one-body equations need to be derived

III. Generator Coordinate Calculations and projection on $J$

* Impact on configuration mixing calculations remains to be seen
* The method needs to be generalized to different "left" $\langle \Phi_L(0) \rangle$ and "right" $\langle \Phi_R(0) \rangle$ vacua