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

<u>HFB</u>

$$|\Phi(\varphi)\rangle = \prod_{\mu>0}(u_\mu + v_{\bar{\mu}}\, e^{2i\varphi}\, a^\dagger_\mu a^\dagger_{\bar{\mu}})|0\rangle$$

Diagonal density matrix and pairing tensor:

$$\rho_{\varphi\,\mu\mu} = \rho_{0\,\mu\mu} = v^2_\mu$$

$$\kappa_{\varphi\,\mu\bar{\mu}} = \kappa_{0\,\mu\bar{\mu}} = u_\mu v_{\bar{\mu}}$$

$$\kappa^*_{\varphi\,\mu\bar{\mu}} = \kappa^*_{0\,\mu\bar{\mu}} = u_\mu v_{\bar{\mu}}$$

Observable are independent of φ:

$$E = \text{"}\,\langle\Phi(0)|H|\Phi(0)\rangle/\langle\Phi(0)|\Phi(0)\rangle\text{"}$$

<u>PNP-HFB</u>

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

Transition density matrix and pairing tensor:

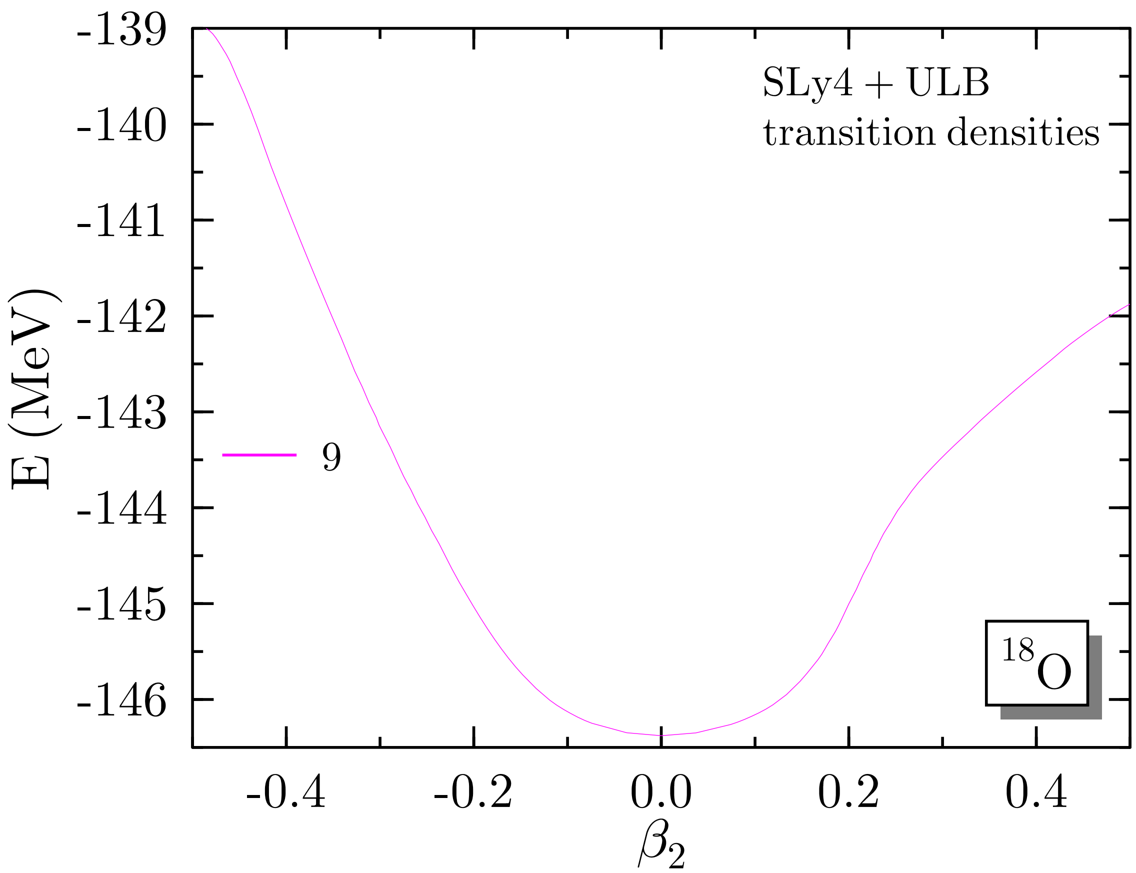
$$\rho_{\mu\mu}(\varphi) = v^2_\mu\, e^{2i\varphi}/(u^2_\mu + v^2_{\bar{\mu}}\, e^{2i\varphi})$$

$$\kappa^{10}_{\mu\bar{\mu}}(\varphi) = u_\mu v_{\bar{\mu}}\, e^{2i\varphi}/(u^2_\mu + v^2_{\bar{\mu}}\, e^{2i\varphi})$$

$$\kappa^{01}_{\mu\bar{\mu}}(\varphi) = u_\mu v_{\bar{\mu}}\,/(u^2_\mu + v^2_{\bar{\mu}}\, e^{2i\varphi})$$

$$E^N = \text{"}\,\langle\Phi(0)|H\hat{P}^N|\Phi(0)\rangle/\langle\Phi(0)|\hat{P}^N|\Phi(0)\rangle\text{"}$$

Problem with PNP-HFB method I



PES: ^{18}O

3D PNP-HFBLN (PAV)

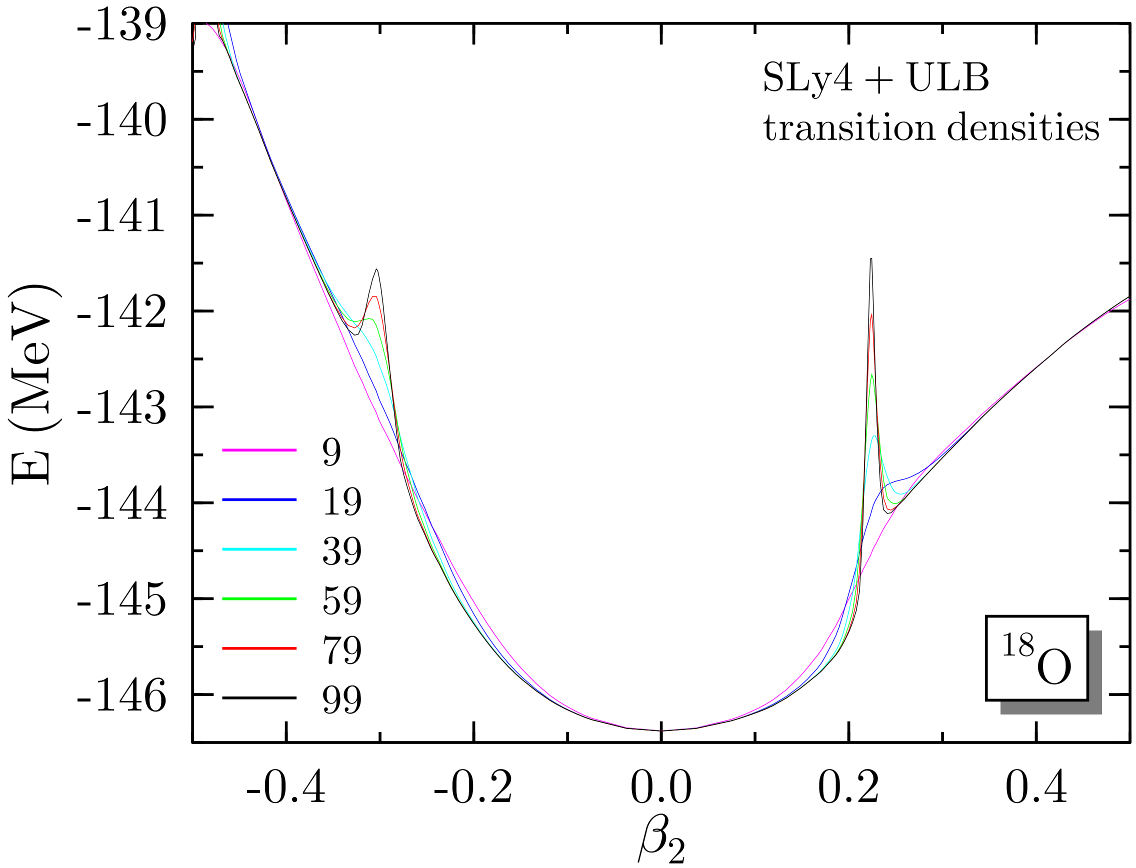
SLy4+ULB

9 φ-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 φ-integration points

*Divergence when a pair of states crosses λ, *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 ρ and κ (bilinear here)

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

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

$$\mathcal{E}^N = \frac{\int_0^{2\pi} d\varphi\, e^{-i\varphi N}\,\mathcal{E}\left[\varphi\right]\,\mathcal{I}(\varphi)}{\int_0^{2\pi} d\varphi\, e^{-i\varphi N}\mathcal{I}(\varphi)} \qquad \text{with} \quad \mathcal{I}(\varphi) = \langle\Phi(0)|\Phi(\varphi)\rangle = \prod_{\nu>0}(u^2_\nu + v^2_\nu\, e^{2i\varphi})$$

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

*$\mathcal{E}\left[\varphi\right]$ 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

	HFB		PNP-HFB	
	$\mathcal{E}\,[\rho, \kappa, \kappa^*]$		$\mathcal{E}\,[\varphi]$	
$\langle \Phi(0) \vert V^{(2)} \vert \Phi(\varphi) \rangle$ (GWT)	$\rho\,\rho\,/\,\kappa^*\,\kappa$	$\longrightarrow$	$\rho(\varphi)\,\rho(\varphi)\,/\,\kappa^{01}(\varphi)\,\kappa^{10}(\varphi)$	
$\langle \Phi(0) \vert V^{(3)} \vert \Phi(\varphi) \rangle$ (GWT)	$\rho\,\rho\,\rho\,/\,\kappa^*\,\kappa\,\rho$	$\longrightarrow$	$\rho(\varphi)\,\rho(\varphi)\,\rho(\varphi)\,/\,\kappa^{01}(\varphi)\,\kappa^{10}(\varphi)\,\rho(\varphi)$	
2-body correl. (MBPT)	$\rho\,\rho\,\rho^{\alpha}$	$\longrightarrow$	$\rho(\varphi)\,\rho(\varphi)\,\rho_0^{\alpha}$	*T. D. (2004)*
Pairing regularization	$\kappa^*\,\kappa\,\rho^{\gamma}$	$\longrightarrow$	$\kappa^{01}(\varphi)\,\kappa^{10}(\varphi)\,\rho_0^{\gamma}$	*T. D. (unpublished)*
Coulomb Exchange (Slater)	$\rho_p\,\rho_p^{1/3}$	$\longrightarrow$	?	

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

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

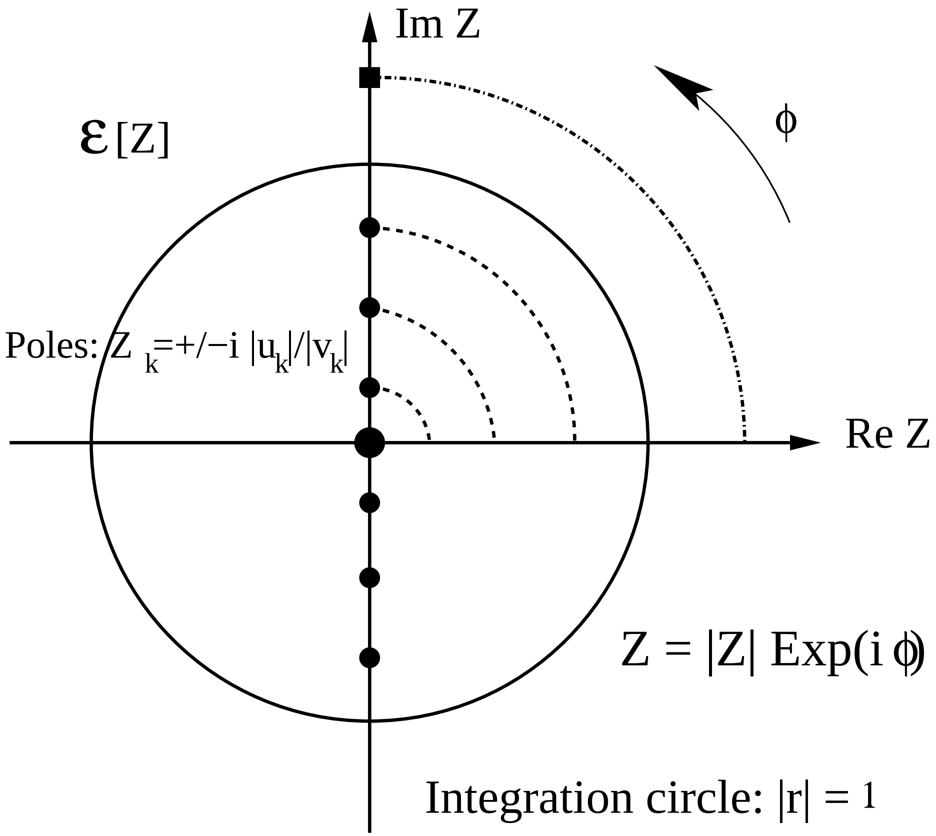
*Potential divergences from terms such that $\nu = \mu, \bar{\mu}$

*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



*$z = e^{i\varphi}$

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

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

*Only $z = 0$ contributes for H

*Divergence in $\mathcal{E}^N$ when poles crosse $\mathcal{C}_1$

*Step left in $\mathcal{E}^N$ after the crossing

*Is that physical?

*Is there a solution to those problems?

Interpretation : self-interaction and self-pairing in DFT

I. HFB

*Self-interaction issue $\mathcal{E}_{\mu} = t_{\mu\mu}\, v_{\mu}^{2} + w^{\rho\rho}_{\mu\mu\mu\mu}\, v_{\mu}^{4} \; \neq \; t_{\mu\mu}\, \rho_{\mu\mu}$

*Self-pairing issue

$$\mathcal{E}_{\mu\bar{\mu}} - (\mathcal{E}_{\mu} + \mathcal{E}_{\bar{\mu}}) \quad = \quad \left(w^{\rho\rho}_{\mu\bar{\mu}\mu\bar{\mu}} + w^{\rho\rho}_{\bar{\mu}\mu\bar{\mu}\mu}\right)\, v_{\mu}^{4} + 4\, w^{\kappa\kappa}_{\mu\bar{\mu}\mu\bar{\mu}}\, u_{\bar{\mu}}^{2}\, v_{\mu}^{2} \; \neq \; \bar{w}^{\rho\rho}_{\mu\bar{\mu}\mu\bar{\mu}}\, \rho^{(2)}_{\mu\bar{\mu}\mu\bar{\mu}}$$

$$\text{where} \quad \rho^{(2)}_{\mu\bar{\mu}\mu\bar{\mu}} = \frac{\langle \Phi(\varphi) | a^{\dagger}_{\mu} a^{\dagger}_{\bar{\mu}} a_{\bar{\mu}} a_{\mu} | \Phi(\varphi) \rangle}{\langle \Phi(\varphi) | \Phi(\varphi) \rangle} = v_{\mu}^{2}$$

*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

$$\mathcal{E}^N_\mu = \int_0^{2\pi} d\varphi \, \frac{e^{-i\varphi N}}{2\pi \, \mathcal{D}_N} \left[t_{\mu\mu} + w^{\rho\rho}_{\mu\mu\mu\mu} \frac{v^2_\mu e^{2i\varphi}}{u^2_\mu + v^2_{\bar\mu} \, e^{2i\varphi}} \right] v^2_\mu \, e^{2i\varphi} \prod_{\nu \neq \mu > 0} (u^2_\nu + v^2_{\bar\nu} \, e^{2i\varphi}) \neq t_{\mu\mu} \, \rho^{\Psi^N}_{\mu\mu}$$

*Self-pairing issue

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

$$\neq \bar{w}^{\rho\rho}_{\mu\bar\mu\mu\bar\mu} \, \rho^{\Psi^N (2)}_{\mu\bar\mu\mu\bar\mu}$$

where $\rho^{\Psi^N (2)}_{\mu\bar\mu\mu\bar\mu} = \frac{\langle \Psi^N | a^\dagger_\mu a^\dagger_{\bar\mu} a_{\bar\mu} a_\mu | \Psi^N \rangle}{\langle \Psi^N | \Psi^N \rangle} = v^2_\mu \int_0^{2\pi} d\varphi \, \frac{e^{-i\varphi N}}{2\pi \, \mathcal{D}_N} \, e^{2i\varphi} \prod_{\nu \neq \mu > 0} (u^2_\nu + v^2_{\bar\nu} \, e^{2i\varphi}) = \rho^{\Psi^N}_{\mu\mu}$

*Pair additive problem

*More dramatic than at the mean-field level

A minimal solution to the problem: motivation from H

*Pair additive problem $\Longrightarrow$ Toy model with only one pair rotated: $\begin{pmatrix} u_\mu(\varphi) \\ v_{\bar{\mu}}(\varphi) \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & e^{2i\varphi} \end{pmatrix} \begin{pmatrix} u_\mu \\ v_{\bar{\mu}} \end{pmatrix}$

$$|\phi(\varphi)\rangle = (u_\mu + v_{\bar{\mu}}\, e^{2i\varphi}\, a^\dagger_\mu a^\dagger_{\bar{\mu}}) \prod_{\nu \neq \mu > 0} (u_\nu + v_{\bar{\nu}}\, a^\dagger_\nu a^\dagger_{\bar{\nu}})|0\rangle = e^{i\varphi} \cos\varphi\, |\phi(0)\rangle - i e^{i\varphi} \sin\varphi\, |\phi(\tfrac{\pi}{2})\rangle$$

*Using the Standard Wick Theorem (SWT)

$$\mathcal{E}_{\rho\rho/\kappa\kappa}(\varphi)_{SWT} = e^{i\varphi} \cos\varphi\; \mathcal{E}_{\rho\rho/\kappa\kappa}(0)_{SWT} - i e^{i\varphi} \sin\varphi\; \mathcal{E}_{\rho\rho/\kappa\kappa}(\tfrac{\pi}{2})_{SWT}$$

*Using the GWT

$$\begin{aligned} \mathcal{E}_{\rho\rho}(\varphi)_{GWT} &= \mathcal{E}_{\rho\rho}(\varphi)_{SWT} + \left(w^{\rho\rho}_{\mu\mu\mu\mu} + w^{\rho\rho}_{\bar{\mu}\bar{\mu}\bar{\mu}\bar{\mu}} + w^{\rho\rho}_{\mu\bar{\mu}\mu\bar{\mu}} + w^{\rho\rho}_{\bar{\mu}\mu\bar{\mu}\mu}\right) u^2_\mu\, v^4_{\bar{\mu}} \frac{e^{2i\varphi}\left(e^{2i\varphi} - 1\right)}{u^2_\nu + v^2_{\bar{\nu}}\, e^{2i\varphi}} \\ \mathcal{E}_{\kappa\kappa}(\varphi)_{GWT} &= \mathcal{E}_{\kappa\kappa}(\varphi)_{SWT} - 4\, w^{\kappa\kappa}_{\mu\bar{\mu}\mu\bar{\mu}}\, u^2_\mu\, v^4_{\bar{\mu}} \frac{e^{2i\varphi}\left(e^{2i\varphi} - 1\right)}{u^2_\nu + v^2_{\bar{\nu}}\, e^{2i\varphi}} \end{aligned}$$

*Spurious terms are directly related to the use of the GWT at finite φ

*Identification of the spurious terms to be removed

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

*Correct dramatic self-interaction/-pairing effects at the PNP-HFB level but not at the HFB level

Spurious contribution to $\mathcal{E}^N$ in realistic PNP-HFB

I. Integration in real space

$$\mathcal{E}^N_{spu.} = \sum_{\mu>0} \left[\left(w^{\rho\rho}_{\mu\mu\mu\mu} + w^{\rho\rho}_{\bar\mu\bar\mu\bar\mu\bar\mu} + w^{\rho\rho}_{\mu\bar\mu\mu\bar\mu} + w^{\rho\rho}_{\bar\mu\mu\bar\mu\mu} \right) - 4\, w^{\kappa\kappa}_{\mu\bar\mu\mu\bar\mu} \right] u^2_\mu v^4_{\bar\mu} \int_0^{2\pi} d\varphi \, \frac{e^{-i\varphi N}}{2\pi \, \mathcal{D}_N} \frac{e^{2i\varphi} \left(e^{2i\varphi} - 1 \right)}{\left(u^2_\mu + v^2_{\bar\mu} \, e^{2i\varphi} \right)^2} \prod_{\nu>0} (u^2_\nu + v^2_{\bar\nu} \, e^{2i\varphi})$$

II. Integration in the complex plane

*Pole at $0 < |z^\pm_\mu| < 1 \Longrightarrow$ remove completely the contribution of the pole to $\mathcal{E}^N$

$$\mathcal{R}e^N_{spu.}(z^\pm_\mu) = - \left(\frac{v_{\bar\mu}}{u_\mu} \right)^N \frac{1 + (-1)^N}{2\, i^N} \prod_{\nu \neq \mu > 0} \frac{u^2_\nu v^2_{\bar\mu} - v^2_\nu u^2_\mu}{v^2_{\bar\mu}}$$

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

$$\mathcal{R}e^2_{spu.}(0)_\mu = -\frac{1}{u^2_\mu} \prod_{\nu \neq \mu > 0} u^2_\nu$$

$$\mathcal{R}e^N_{spu.}(0)_\mu = -\frac{v^2_{\bar\mu}}{u^2_\mu} \mathcal{R}e^{N-2}_{spu.}(0)_\mu + \frac{1}{u^2_\mu} \left[\sum_{\{\lambda\}_{n-2}} \prod_{\substack{\nu \neq \\ \mu, \{\lambda\}}} u^2_\nu \prod_{\{\lambda\}} v^2_{\bar\lambda} - \sum_{\{\lambda\}_{n-1}} \prod_{\substack{\nu \neq \\ \mu, \{\lambda\}}} u^2_\nu \prod_{\{\lambda\}} v^2_{\bar\lambda} \right]$$

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" $\langle \Phi_L(0)|$ and "right" $|\Phi_R(0)\rangle$ vacua