Regularization Scheme Applied to Particle Number Projection in MR Functional Theory

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Particle mixing

In HFB theory, the Bogoliubov transformation

$$\begin{pmatrix} \beta \\ \beta^\dagger \end{pmatrix} = \begin{pmatrix} U^\dagger & V^\dagger \\ V^T & U^T \end{pmatrix} \begin{pmatrix} c \\ c^\dagger \end{pmatrix}$$

defines the quasi-particle operators β and $\beta^\dagger$ as combination of the single particle operators c and $c^\dagger$.

The HFB equations produce solutions in which the single-particle operators are mixed.
$\Rightarrow$ The ground state wave function does not have a defined number of particles.

$\Rightarrow$ Restoration of the number of particles symmetry in the multireference EDF.

Projector over the number of particles N (neutrons)

$$\hat{P}_N = \frac{1}{2\pi} \int_0^{2\pi} d\phi \, e^{i\,\phi\,(\hat{N}-N)}$$

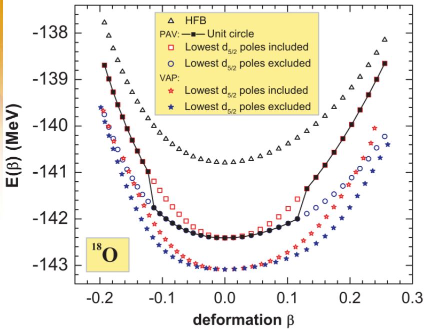
In the HFODD solver, this integration is performed by discretization

$$\int d\phi \, e^{-i\,\phi\,N} \ldots \rightarrow \frac{1}{L} \sum_{k=1}^{L} e^{-i\,\frac{2\pi k}{L}\,N} \ldots$$

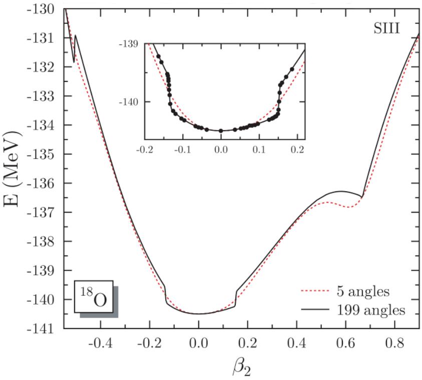
(**V.N. Fomenko, J. Phys. A 3 (1970) 8**)
where L is the number of points used to represent the gauge angle ϕ in the complex plane.

Problems related with Particle Number Projection PNP

- poles along the imaginary axis
- dependence on the contour of integration
- fractional power of ρ



J. Dobaczewski et al., Phys. Rev. C 76 (2007) 054315



M. Bender et al., Phys. Rev. C 79 (2009) 044319

The simple regularization for the Angular Momentum Projection in **W. Satuła and J. Dobaczewski, Phys. Rev. C 90 (2014) 054303** is extended to the Particle Number Projection (Projection After Variation) of the energy

$$E_N = \frac{\frac{1}{2\pi}\int_0^{2\pi} d\phi\, e^{-i\phi N}\ \varepsilon[\rho,\bar{\rho}](\phi)\ \langle\Psi|\Psi(\phi)\rangle}{\frac{1}{2\pi}\int_0^{2\pi} d\phi\, e^{-i\phi N}\ \langle\Psi|\Psi(\phi)\rangle}$$

Basic steps for the regularization:

- ⋆ canonical wave functions solutions of HFB equations ⇒ gauge rotated wave functions, densities and Skyrme functionals
  - ε functional of the total energy
  - $\langle\Psi|\Psi(\phi)\rangle$ overlap between initial and gauge-rotated wave functions

- expansion of the overlap (regular)

$$\langle \Psi | \Psi(\phi) \rangle = \sum_{R=-\infty}^{+\infty} c_R \, e^{i\phi R}$$

with coefficients

$$c_R = \frac{1}{2\pi} \int_0^{2\pi} d\phi \, e^{-i\phi R} \, \langle \Psi | \Psi(\phi) \rangle$$

- auxiliary energy

$$E_{N,1} = \frac{1}{c_N} \frac{1}{2\pi} \int_0^{2\pi} d\phi \, e^{-i\phi N} \, \varepsilon[\rho, \bar{\rho}](\phi) \, \langle \Psi | \Psi(\phi) \rangle \langle \Psi | \Psi(\phi) \rangle$$

- assumed regular matrix elements

$$\widetilde{\langle \varepsilon \rangle} = \widetilde{\varepsilon}[\rho, \bar{\rho}](\phi) \, \langle \Psi | \Psi(\phi) \rangle = \sum_{K=-\infty}^{+\infty} \widetilde{\langle \varepsilon_K \rangle} \, e^{i\phi K}$$

⋆ matrix of coefficients $(C)_{NK}$

$$\sum_K (C)_{NK} \, \widetilde{\langle \varepsilon_K \rangle} = c_N \, E_{N,1}$$

to be inverted to obtain the regularized projected energies

$$\widetilde{E}_N = \frac{1}{c_N} \widetilde{\langle \varepsilon_N \rangle}$$

⋆ sum rule to check that the sum of the all projected energies gives back the initial energy

$$E = \sum_N \langle \Psi_N | \Psi_N \rangle \, \widetilde{E}_N = \sum_N \widetilde{\langle \varepsilon_N \rangle}$$

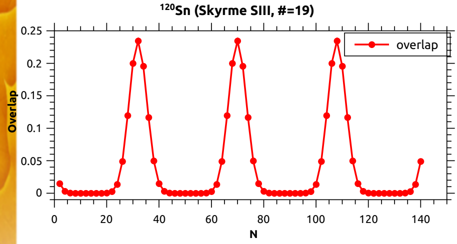
Technical difficulties

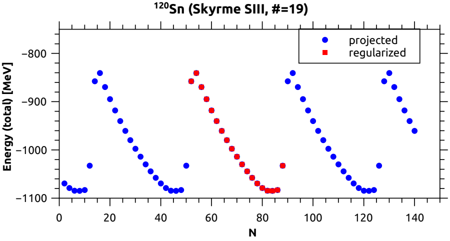
Inversion made by Singular Value Decomposition method:
restricted only on M x M matrix to have linear independent row or column in C_{NK}
M $= min(N, L)$.
The projection operator is periodic

$$e^{-i\,\frac{2\pi k}{L}\,N} = e^{-i\,\frac{2\pi k}{L}\,N+L}$$

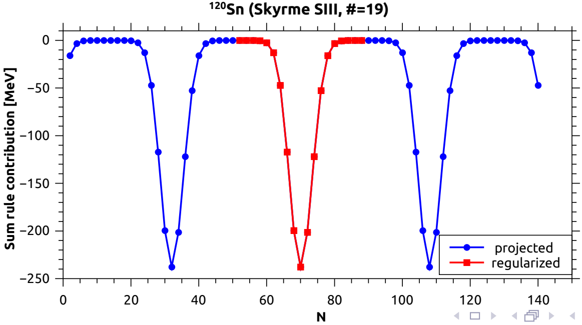
The sum rule runs over a number of different N equal to M instead of from $-\infty$ to $+\infty$

Periodicity of overlap and total energy (projected)

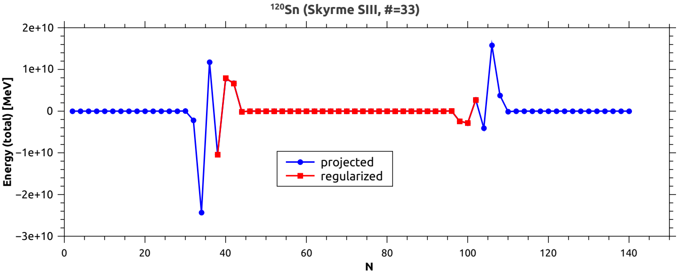


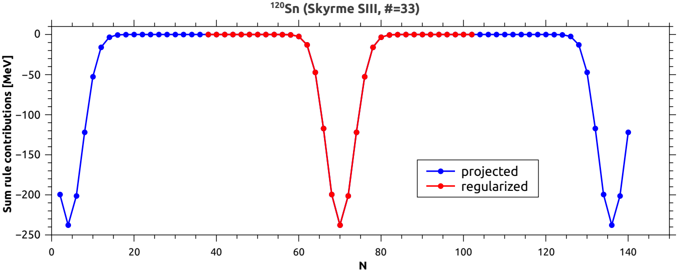


Sum rule contributions

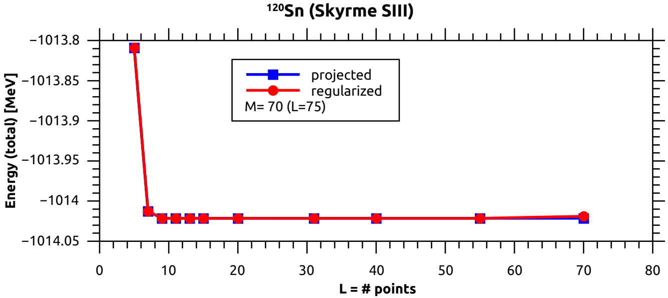


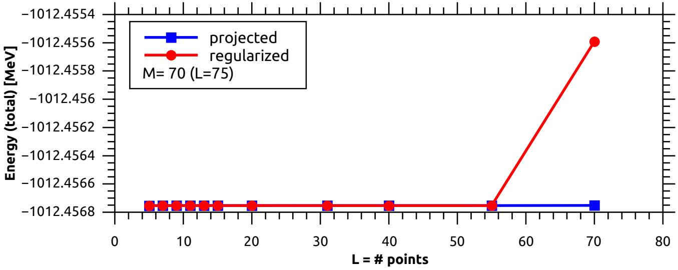
Fluctuation of the projected energy far from the expected value $\langle N \rangle$



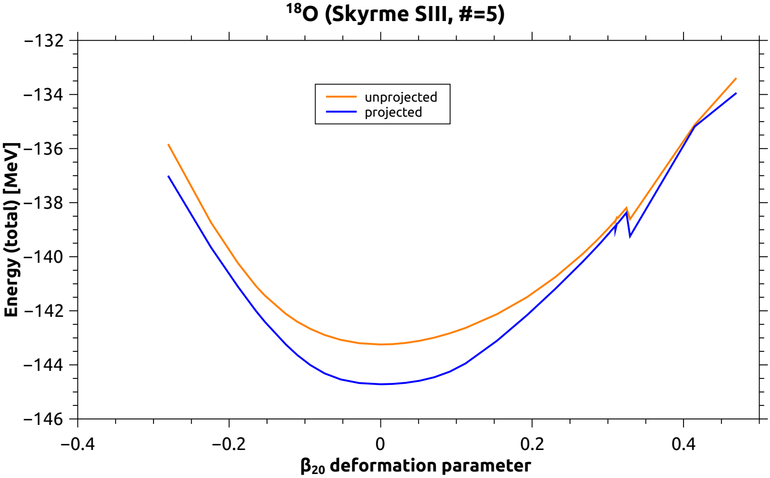


(No) differences between PNP and regularized PNP



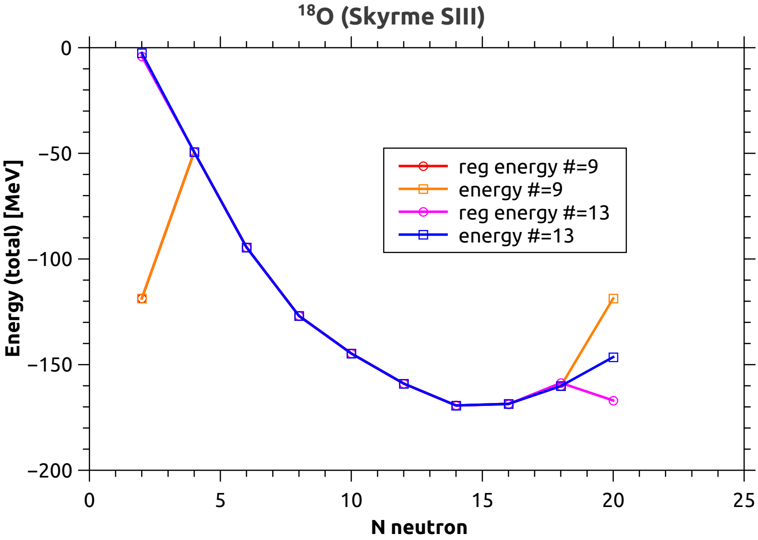


Energy behaviour as function of β_{20} deformation parameter



Future development:

- new tests to figure out improvement of the regularization
- simultaneous projection on neutron and proton number



^{18}O (Skyrme SIII)
Energy (total) [MeV]
N neutron
0
−50
−100
−150
−200
0
5
10
15
20
25
reg energy #=9
energy #=9
reg energy #=13
energy #=13