Particle–Number Projected HFB Method with Skyrme Forces

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Theoretical Description of the Nuclear Large Amplitude Collective Motion, Oak Ridge, March 30-31, 2005

HFB Method

\[ H = \sum_{n_1n_2} e_{n_1n_2} c_{n_1}^\dagger c_{n_2} + \frac{1}{4} \sum_{n_1n_2n_3n_4} \bar{v}_{n_1n_2n_3n_4} c_{n_1}^\dagger c_{n_2}^\dagger c_{n_3} c_{n_4}, \]

\[ \bar{v}_{n_1n_2n_3n_4} = \langle n_1n_2|V|n_3n_4 - n_4n_3\rangle, \quad c_n|\rightarrow\rangle = 0. \]

\[
\begin{pmatrix}
\alpha \\
\alpha^\dagger
\end{pmatrix} =
\begin{pmatrix}
U^\dagger & V^\dagger \\
V^T & U^T
\end{pmatrix}
\begin{pmatrix}
c \\
c^\dagger
\end{pmatrix}
\]

\[ \alpha_k|\Phi\rangle = 0, \quad \hat{N}|\Phi\rangle \neq N|\Phi\rangle \]

\[ \rho_{n'\bar{n}} = \frac{\langle \Phi | c_{n'}^\dagger c_{n'} | \Phi \rangle}{\langle \Phi | \Phi \rangle}, \quad \tilde{\rho}_{n'\bar{n}} = \frac{\langle \Phi | s_{\bar{n}}^* c_{n'} | \Phi \rangle}{\langle \Phi | \Phi \rangle}, \]

\[ \hat{T}\phi_n(r, \sigma) = s_n\phi_n(r, \sigma), \quad s_n s_n^* = 1, \quad s_{\bar{n}} = -s_n \]

\[ E[\rho, \tilde{\rho}] = \frac{\langle \Phi | H | \Phi \rangle}{\langle \Phi | \Phi \rangle} \]

\[
\begin{pmatrix}
h - \lambda & \tilde{h} \\
\tilde{h} & -h + \lambda
\end{pmatrix}
\begin{pmatrix}
U \\
V
\end{pmatrix}_k = E_k
\begin{pmatrix}
U \\
V
\end{pmatrix}_k
\]

\[ h_{nn'} = \frac{\partial E[\rho, \tilde{\rho}]}{\partial \rho_{n'n}}, \quad \tilde{h}_{nn'} = \frac{\partial E[\rho, \tilde{\rho}]}{\partial \tilde{\rho}_{n'n}} \]
Particle Number Projected HFB Method

Projection After Variation (PAV)

\[ E_{HFB} = \frac{\langle \Phi | H | \Phi \rangle}{\langle \Phi | \Phi \rangle}, \quad \hat{N} | \Phi \rangle \neq N | \Phi \rangle \]

\[ P^N = \frac{1}{2\pi} \int d\phi \ e^{i\phi(\hat{N} - N)} \]

\[ |\Psi^N\rangle = P^N | \Phi \rangle, \quad \hat{N} |\Psi^N\rangle = N |\Psi^N\rangle \]

\[ E_{PAV}^N = \frac{\langle \Psi^N | H | \Psi^N \rangle}{\langle \Psi^N | \Psi^N \rangle} = \frac{\langle \Phi | H P^N | \Phi \rangle}{\langle \Phi | P^N | \Phi \rangle} \]

\[ E_{HFB} \quad 2-3 \text{ MeV} \]

\[ E_{PAV}^N \]
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**Particle Number Projected HFB Method**

Variation After Projection (VAP)

\[
E^N_{HFB} = 2-3 \text{ MeV}
\]

\[
E^N_{PAV} = \sim 1 \text{ MeV}
\]

\[
E^N_{HFB} = \left( \frac{\phi | H P^N | \phi}{\phi | P^N | \phi} \right) = \frac{\int d\phi \langle \phi | H e^{i\phi(\bar{N}-N)} | \phi \rangle}{\int d\phi \langle \phi | e^{i\phi(\bar{N}-N)} | \phi \rangle}
\]

\[
\begin{pmatrix}
\varepsilon^N + \Gamma^N + \Lambda^N \\
-(\Delta^N)^* 
\end{pmatrix}
\begin{pmatrix}
\Delta^N \\
-(\varepsilon^N + \Gamma^N + \Lambda^N)^*
\end{pmatrix}
= \begin{pmatrix} U \\ V \end{pmatrix}_k = E^N_k \begin{pmatrix} U \\ V \end{pmatrix}_k
\]

\[
\varepsilon^N = \frac{1}{2} \int d\phi \ y(\phi) \left( Y(\phi) Tr[e\rho(\phi)] + [1 - 2ie^{-i\phi}\sin\phi\rho(\phi)]eC(\phi) \right) + h.c.
\]

\[
\Gamma^N = \frac{1}{4} \int d\phi \ y(\phi) \left( Y(\phi) Tr[\Gamma(\phi)\rho(\phi)] + 2[1 - 2ie^{-i\phi}\sin\phi\rho(\phi)]\Gamma(\phi)C(\phi) \right) + h.c.
\]

\[
\Lambda^N = -\frac{1}{4} \int d\phi \ y(\phi) \left( Y(\phi) Tr[\Delta(\phi)\kappa^*(\phi)] - 4ie^{-i\phi}\sin\phi\ C(\phi)\Delta(\phi)\kappa^*(\phi) \right) + h.c.
\]

\[
\Gamma_{n1n3}(\phi) = \sum_{n2n4} \bar{v}_{n1n2n3n4} \rho_{n4n2}(\phi),
\]

\[
\Delta^N = \frac{1}{2} \int d\phi \ e^{-2i\phi} C(\phi) \Delta(\phi) - (..)^T,
\]

\[
\Delta_{n1n2}(\phi) = \frac{1}{2} \sum_{n3n4} \bar{v}_{n1n2n3n4} \kappa_{n3n4}(\phi), \quad \Delta^*_{n3n4}(\phi) = \frac{1}{2} \sum_{n1n3} \kappa_{n1n2}(\phi) v_{n1n2n3n4},
\]

\[
\rho(\phi) = C(\phi)\rho \quad \kappa(\phi) = (\phi)\kappa = \kappa^{T}(\phi)
\]

\[
\bar{\kappa}(\phi) \quad e^{2i\phi}\kappa^{*}(\phi) = e^{2i\phi}C^{t}(\phi)\kappa
\]

\[
C(\phi) = e^{2i\phi} \left( 1 + \rho(e^{2i\phi} - 1) \right)^{-1},
\]

\[
x(\phi) = \frac{1}{2\pi} \frac{e^{-i\phi N} \det(e^{i\phi}I)}{\sqrt{\det C(\phi)}}, \quad y(\phi) = \frac{x(\phi)}{\int d\phi' x(\phi')}, \quad \int d\phi \ y(\phi) = 1.
\]
Skyrme HFB Method

\[ \frac{\langle \Phi | H | \Phi \rangle}{\langle \Phi | \Phi \rangle} \rightleftharpoons E[\rho, \tilde{\rho}] = \int dr \left[ H(r) + \tilde{H}(r) \right] \]

\( H(r) \) and \( \tilde{H}(r) \) are normal and pairing energy densities, respectively, expressed in terms of particle and pairing local densities and currents.

\[ \rho(r_\sigma, r'_\sigma') = \sum_{nn'} \rho_{nn'} \psi^*_n(r'_\sigma, \sigma') \psi_n(r, \sigma) \]

\[ \tilde{\rho}(r_\sigma, r'_\sigma') = \sum_{nn'} \tilde{\rho}_{nn'} \psi^*_n(r'_\sigma, \sigma') \psi_n(r, \sigma) \]

\[ h_{nn'} = \frac{\partial E[\rho, \tilde{\rho}]}{\partial \rho_{n'n}}, \quad \tilde{h}_{nn'} = \frac{\partial E[\rho, \tilde{\rho}]}{\partial \tilde{\rho}_{n'n}} \]

\[ \left( \begin{array}{cc} h - \lambda & \tilde{h} \\ \tilde{h} & -h + \lambda \end{array} \right) \left( \begin{array}{c} U \\ V \end{array} \right)_k = E_k \left( \begin{array}{c} U \\ V \end{array} \right)_k \]
PNP Skyrme HFB Method

\[ E[\rho, \tilde{\rho}] \leftrightarrow \langle \Phi | \hat{H} | \Phi \rangle \]

Densities \( \rho, \tilde{\rho} \) associated with a single state \( |\Phi\rangle \)

\[ E^N[\rho, \tilde{\rho}] \leftrightarrow \frac{\langle \Phi | H P^N | \Phi \rangle}{\langle \Phi | P^N | \Phi \rangle} \]

Requires knowledge of off-diagonal expectation values which are not automatically given by DFT

\[ \langle \Phi(0) | \hat{H} | \Phi(\varphi) \rangle, \quad |\Phi(\varphi)\rangle = e^{\varphi(N-N)} |\Phi\rangle \]

‘Mixed Densities’ Prescription

Obviously certain extensions are necessary and they are not unique. Among various possibilities, the so-called ‘mixed density’ recipe is most frequently used in projection and other GCM calculations.

\[ \rho(\varphi) = \langle \Phi(0) | \hat{\rho} | \Phi(\varphi) \rangle, \quad \tilde{\rho}(\varphi) = \langle \Phi(0) | \hat{\tilde{\rho}} | \Phi(\varphi) \rangle \]
PNP Skyrme HFB Method

Energy Functional under ‘Mixed densities’ prescription

\[ E^N[\rho, \tilde{\rho}] = \frac{\int d\varphi \ e^{-\varphi N} \mathcal{I}(\varphi) \ E[\rho(\varphi), \tilde{\rho}(\varphi)]}{\int d\varphi \ e^{-\varphi N} \mathcal{I}(\varphi)} = \int d\varphi \ y(\varphi) \ E[\rho(\varphi), \tilde{\rho}(\varphi)] \]

\[ y(\varphi) = \frac{e^{\varphi N} \mathcal{I}(\varphi)}{\int d\varphi \ e^{-\varphi N} \mathcal{I}(\varphi)}, \quad \int d\varphi \ y(\varphi) = 1, \quad \mathcal{I}(\varphi) = \langle \Phi(0) | \Phi(\varphi) \rangle \]

\[ \rho(\varphi) = \langle \Phi(0) | \hat{\rho} | \Phi(\varphi) \rangle, \quad \tilde{\rho}(\varphi) = \langle \Phi(0) | \hat{\tilde{\rho}} | \Phi(\varphi) \rangle \]

\[ E[\rho(\varphi), \tilde{\rho}(\varphi)] = \int d\mathbf{r} \mathcal{H}(\mathbf{r}, \phi) \]

- \( \rho(\mathbf{r}), \tilde{\rho}(\mathbf{r}) \longrightarrow \rho(\mathbf{r}, \phi), \tilde{\rho}(\mathbf{r}, \phi) \)
- \( \tau(\mathbf{r}), \tilde{\tau}(\mathbf{r}) \longrightarrow \tau(\mathbf{r}, \phi), \tilde{\tau}(\mathbf{r}, \phi) \)
- \( \mathbf{J}_{ij}(\mathbf{r}), \tilde{\mathbf{J}}_{ij}(\mathbf{r}) \longrightarrow \mathbf{J}_{ij}(\mathbf{r}, \phi), \tilde{\mathbf{J}}_{ij}(\mathbf{r}, \phi) \)

Canonical Representation

Unprojected density
\[ \rho_n = v_n^2, \quad \tilde{\rho}_n = u_n v_n \]  
\[ \mathcal{I}(\varphi) = \prod_n \left( \frac{u_n^2 + v_n^2 \ e^{2\varphi}}{u_n^2 + v_n^2 \ e^{2\varphi}} \right) \]

‘Mixed’ density
\[ \rho_n(\varphi) = \frac{v_n^2 \ e^{2\varphi}}{u_n^2 + v_n^2 \ e^{2\varphi}}, \quad \tilde{\rho}_n(\varphi) = \frac{u_n v_n \ e^{\varphi}}{u_n^2 + v_n^2 \ e^{2\varphi}} \]

Projected density
\[ \rho^N_n = \int d\varphi \ y(\varphi) \rho_n(\varphi), \quad \tilde{\rho}^N_n = \int d\varphi \ y(\varphi) \tilde{\rho}_n(\varphi) \]
PNP Skyrme HFB Method

VAP under ‘Mixed densities’ prescription

\[
\begin{pmatrix} h^N & \tilde{h}^N \\ \tilde{h}^N & -h^N \end{pmatrix} \begin{pmatrix} U \\ V \end{pmatrix}_k = E_k^N \begin{pmatrix} U \\ V \end{pmatrix}_k
\]

\[
h^N = \int d\phi y(\phi)Y(\phi)E(\phi) + \int d\phi y(\phi)e^{-2i\phi} C(\phi)\tilde{h}(\phi)C(\phi)
- [ \int d\phi y(\phi)2ie^{-i\phi}\sin(\phi)\tilde{\rho}(\phi)\tilde{h}(\phi)C(\phi) + h.c.] ,
\]

\[
\tilde{h}^N = \int d\phi y(\phi)e^{-i\phi}(\tilde{h}(\phi)C(\phi) + (...)^T)
\]

\[
h(\phi) = \frac{\partial E[\rho(\phi), \tilde{\rho}(\phi)]}{\partial \rho(\phi)}, \quad \tilde{h}(\phi) = \frac{\partial E[\rho(\phi), \tilde{\rho}(\phi)]}{\partial \tilde{\rho}(\phi)}
\]

\[
\rho_n = v_n^2, \quad \tilde{\rho}_n = u_nv_n, \quad \rho_n(\varphi) = \frac{v_n^2e^{2i\varphi}}{u_n^2 + v_n^2e^{2i\varphi}}, \quad \tilde{\rho}_n(\varphi) = \frac{u_nv_ne^{i\varphi}}{u_n^2 + v_n^2e^{2i\varphi}}
\]

\[
C_{\mu}(\phi) = \frac{e^{2i\phi}}{u_{\mu}^2 + e^{2i\phi}v_{\mu}^2}, \quad y(\phi) = \frac{e^{-iN\phi}}{\sum_{l=0}^{L-1} e^{-iN\phi_l} \prod_{\mu>0} (u_{\mu}^2 + e^{2i\phi_l}v_{\mu}^2)}
\]

\[
Y_{\mu}(\phi) = ve^{-i\phi}\sin \phi C_{\mu}(\phi) - \sum_{l'=0}^{L-1} Y(\phi_{l'}) ve^{-i\phi_{l'}}\sin \phi_{l'} C_{\mu}(\phi_{l'})
\]

\[
P^N = \frac{1}{2\pi} \int d\phi e^{i\phi(\tilde{N}-N)} \implies P^N = \frac{1}{L} \sum_{l=1}^{L} e^{i\phi_l(\tilde{N}-N)}, \quad \phi_l = \frac{2\pi}{L}(l-1)
\]
PNP Skyrme HFB Method

Problems: Stability

Slow (even unstable) procedure
\[
\begin{pmatrix}
  h^N & \tilde{h}^N \\
  \tilde{h}^N & -h^N
\end{pmatrix}
\begin{pmatrix}
  U \\
  V
\end{pmatrix}
= E_k^N
\begin{pmatrix}
  U \\
  V
\end{pmatrix}

\text{Tr} \rho = \tilde{N}, \quad \rho = V^* V^T
\]

Stable procedure
\[
\begin{pmatrix}
  h^N - \mu & \tilde{h}^N \\
  \tilde{h}^N & -(h^N - \mu)
\end{pmatrix}
\begin{pmatrix}
  U \\
  V
\end{pmatrix}
= E_k^N
\begin{pmatrix}
  U \\
  V
\end{pmatrix}

\text{Tr} \rho = \tilde{N}, \quad \rho = V^* V^T
\]

\[\mu \text{ is zero when the PNP solution is found}\]

\[
\text{Tr} \rho^N = N, \quad \rho^N = \int d\phi y(\phi) C(\phi) \rho
\]
PNP Skyrme HFB Method

Problems: Cut-off procedure for Delta pairing forces

\[ \bar{e}_n = (1 - 2P_n)E_n + \lambda \]
\[ \bar{\Delta}_n = 2E_n\sqrt{P_n(1 - P_n)} \]

Unprojected HFB \( h \) and \( \tilde{h} \) appear in the PNP scheme at gauge angle \( \varphi = 0 \)

\[ \tilde{E}_n = \begin{pmatrix} U \\ V \end{pmatrix}_n \begin{pmatrix} h - \lambda & \tilde{h} \\ \tilde{h} & -h + \lambda \end{pmatrix} \begin{pmatrix} U \\ V \end{pmatrix}_n \]
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PNP Skyrme HFB Method

Problems: Pairing Strength

In the standard Skyrme HFB method the pairing strength \( V_0 \) is chosen in such a way that the HFB value of the average neutron gap \( \tilde{\Delta}_n \) at given cut-off energy \( \epsilon_{\text{cut}} \) reproduces the experimental value 1.245 MeV for the nucleus \(^{120}\text{Sn}\).

The average neutron gap \( \tilde{\Delta}_n \) is no more defined within PNP HFB method. Therefore, the above procedure for adjusting the pairing strength is no more applicable.

A strict way of adjusting the pairing strength should be obtained by calculating mass differences and comparing with available experimental data.

We adjust the pairing strength to the total energy of some nucleus already calculated in PLN HFB approximation. This is rather crude approximation we are using just to analize the quality of the PNP HFB treatment.

\[
\hat{H}(\mathbf{r}) = \frac{1}{2} V_0 \left[ 1 - V_1 \left( \frac{\rho}{\rho_0} \right)^\gamma \right] \sum_q \rho_q^2
\]

\[
V_1 = \begin{cases} 
0 & \text{vouume pairing} \\
1 & \text{surface pairing} 
\end{cases}
\]

\[
\gamma = 1, \quad \rho_0 = 0.16 \text{ fm}^{-3}
\]
PNP Skyrme HFB Method

Ca Chain Calculations

- SLY4 + mixed delta pairing forces
- HFB within 20 major HO shells
- Complete Ca chain
- Comparison:
  - HFB+LN results (LN)
  - PAV HFB+LN results (PLN)
  - VAP PNP HFB results (PNP)
- PLN pairing strength fitted to $\Delta_n$ @ $^{120}$Sn
- PNP pairing strength to PLN $E_{\text{tot}}$ @ $^{44}$Ca

- With L=9 gauge-angle points
  the code is just 9 times slower
PNP Skyrme HFB Method

Some Results

- LN method should be avoided
  - One should use PLN instead
- PLN is a good approximation for open shell nuclei
  - total energy differences are less than 250 KeV
- PLN is wrong for closed shell nuclei
  - total energy differences could be more than 1 MeV
- One should try to correct PLN by projecting from neighboring nuclei
PNP within DFT

Well Known Singularity

\[ \rho_n(\varphi) = \frac{v_n^2 e^{2u\varphi}}{u_n^2 + v_n^2 e^{2u\varphi}} , \quad \tilde{\rho}_n(\varphi) = \frac{u_n v_n e^{u\varphi}}{u_n^2 + v_n^2 e^{2u\varphi}} \]

\[ u_n^2 = v_n^2 = \frac{1}{2}, \quad \varphi = \frac{\pi}{2} \]

We have found in mass table calculations that among all 5818 nuclei only about 50 of them have a neutron state with occupation 0.5 and other 48 nuclei with such a proton state. Therefore, we have about 100 questionable nuclei among 5818 which makes less than 2 percents. The situations however is much more serious when performing constrained HFB calculations.
PNP HFB Method

Shift invariance and Energy sum rule

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

\[ (P^N)^\dagger = P^N, \quad (P^N)^2 = P^N, \quad \sum_N P_N = 1 \]

\[ |\tilde{\Psi}_N \rangle = \frac{\Psi_N}{\sqrt{\langle \Psi_N | \Psi_N \rangle}}, \quad |\tilde{\Phi} \rangle = \frac{\Phi}{\sqrt{\langle \Phi | \Phi \rangle}}, \quad |\tilde{\Phi} \rangle = \sum_N b_N |\tilde{\Psi}_N \rangle, \]

\[ b_N^2 = \frac{\langle \Phi | P_N | \Phi \rangle}{\langle \Phi | \Phi \rangle}, \quad \sum_N |b_N|^2 = 1 \]

\[ E_{HFB} = \frac{\langle \Phi | \hat{H} | \Phi \rangle}{\langle \Phi | \Phi \rangle}, \quad E^N = \frac{\langle \Psi_N | \hat{H} | \Psi_N \rangle}{\langle \Psi_N | \Psi_N \rangle} \]

Shift Invariance

\[ e^{\eta (\hat{N} - N)} |\Psi_N \rangle = |\Psi_N \rangle, \quad \hat{N} |\Psi_N \rangle = N |\Psi_N \rangle \]

Energy Sum Rule

\[ E_{HFB} = \sum_N |b_N|^2 E^N \]

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PNP within DFT

Broken Shift Invariance

Spherical Nuclei

Deformed Nuclei

\[ 1\text{s}_{1/2}, 1\text{p}_{1/2}, 1\text{d}_{5/2}, 1\text{f}_{5/2}, 2\text{s}_{1/2}, 1\text{d}_{3/2}, 1\text{f}_{7/2}, 2\text{p}_{1/2} \]

\[ ^{16}\text{O, SIII, volume pairing, } \beta = -0.79 \]
PNP within DFT

\[ E^N[\rho, \bar{\rho}] = \frac{\int d\varphi \ e^{-\nu^N I(\varphi)} E[\rho(\varphi), \bar{\rho}(\varphi)]}{\int d\varphi \ e^{-\nu^N I(\varphi)}} \]

\[ I(\varphi) = \langle \Phi(0)|\Phi(\varphi) \rangle = \prod_n (u_n^2 + v_n^2 e^{2\nu \varphi}) \]

\[ \rho_n(\varphi) = \frac{v_n^2 e^{2\nu \varphi}}{u_n^2 + v_n^2 e^{2\nu \varphi}}, \quad \bar{\rho}_n(\varphi) = \frac{u_n v_n e^{\nu \varphi}}{u_n^2 + v_n^2 e^{2\nu \varphi}} \]

\[ z = e^{\nu \varphi}, \quad d\varphi = \frac{dz}{iz}, \quad C_1(|z| = 1) \quad \rho_n(z) = \frac{v_n^2 z^2}{u_n^2 + v_n^2 z^2}, \quad \bar{\rho}_n(z) = \frac{u_n v_n z}{u_n^2 + v_n^2 z^2} \]

\[ N_N \equiv \int d\varphi \ e^{-\nu^N I(\varphi)} E[\rho(\varphi), \bar{\rho}(\varphi)] = -i \oint \frac{dz}{z^{N+1}} \prod_n (u_n^2 + v_n^2 z^2) E[\rho(z), \bar{\rho}(z)] \]

\[ D_N \equiv \int d\varphi \ e^{-\nu^N I(\varphi)} = \oint \frac{dz}{z^{N+1}} \prod_n (u_n^2 + v_n^2 z^2) \]

\[ \int_C dz f(z) = 2\pi i \sum_k \text{Res}[f(z_k)] \quad z_k = \pm i \frac{|u_k|}{|v_k|} \]

\[ N_N = 2\pi i \sum_{|z_k| \leq 1} \text{Res} \left[ \frac{1}{z_k^{N+1}} \prod_n (u_n^2 + v_n^2 z_k^2) E[z_k] \right] \]

\[ D_N = 2\pi i \text{Res} \left[ \frac{1}{z_0^{N+1}} \prod_n (u_n^2 + v_n^2 z_0^2) \right] \]
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**PNP within DFT**

**PNP Energy**

\[ E_N = E_N[z_0] + \Delta E_N \]

\[ E_N[z_0] = \frac{\text{Rez} \left[ \frac{1}{z_0^{N+1}} \prod_n \left( \frac{u_n^2 + v_n^2 z_0^2}{u_n^2 + v_n^2 z_0^2} \right) E[z_0] \right]}{\text{Rez} \left[ \frac{1}{z_0^{N+1}} \prod_n \left( \frac{u_n^2 + v_n^2 z_0^2}{u_n^2 + v_n^2 z_0^2} \right) \right]} \]

\[ \Delta E_N = \frac{2\pi n}{D_N} \sum_{0<|z_k|\leq 1} \text{Rez} \left[ \prod_n \left( \frac{u_n^2 + v_n^2 z_k^2}{u_n^2 + v_n^2 z_k^2} \right) \frac{E[z_k]}{z_k^{N+1}} \right] \]

**PNP Energy – explicit pole dependence**

- \( E[\rho, \tilde{\rho}] \) leads to \( f_a(z) \) without pole at \( z_k \)
- \( a = d + p, d \) power of \( \rho, p \) power of \( \tilde{\rho} \)
- \( \nu_k \) is the degeneracy of the \( k \)-th canonical state
  - for deformed nuclei always \( \nu_k = 1 \)
  - for spherical nuclei \( \nu_k = (2j + 1)/2 \)
  - \( \nu_k = 1 \) for \( j = 1/2 \), \( \nu_k = 2 \) for \( j = 3/2 \) ...

\[ E_N = E_N[z_0] + \Delta E_N \]

\[ \Delta E_N = \sum_{0<|z_k|\leq 1} \sum_a \text{Rez} \left[ \frac{(u_k^2 + v_k^2 z_k^2)^{\nu_k} f_a(z_k)}{z_k^{N+1} (u_k^2 + v_k^2 z_k^2)^a} \right] \]

**Shifted PNP Energy**

\[ \frac{\varepsilon^{\eta(N-N)} \Psi_N}{\hat{S}_\eta} \]

\[ C_1(|z| = 1) \Rightarrow C_\eta(|z| = e^{-\eta}) \]

\[ E_N(\eta) = E_N[z_0] + \Delta E_N(\eta) \]

\[ \Delta E_N(\eta) = \sum_{|z_k|\leq e^{-\eta}} \sum_a \text{Rez} \left[ \frac{(u_k^2 + v_k^2 z_k^2)^{\nu_k} f_a(z_k)}{z_k^{N+1} (u_k^2 + v_k^2 z_k^2)^a} \right] \]
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PNP within DFT

Local Shift Invariance

\[ E_N(\eta) = E_N[z_0] + \Delta E_N(\eta) \]
\[ z_0 = 0, \quad z_k = \pm i |u_k/v_k| \leftrightarrow u_k^2 = v_k^2 = \frac{1}{2}, \quad \varphi = \frac{\pi}{2} \]

\[ E_N[z_0] = \frac{\text{Rez} \left[ \frac{1}{z_0^{N+1}} \prod_{n} (u_n^2 + v_n^2 z_0^2) E[z_0] \right]}{\text{Rez} \left[ \frac{1}{z_0^{N+1}} \prod_{n} (u_n^2 + v_n^2 z_0^2) \right]} \]

\[ \Delta E_N(\eta) = \sum_{|z_k| \leq e^{-\eta}} \sum_{a} \text{Rez} \left[ \frac{(u_k^2 + v_k^2 z_k^2)^\eta f_a(z_k)}{z_k^{N+1} (u_k^2 + v_k^2 z_k^2)^a} \right] \]

Spherical Nuclei

\[ \beta = -0.79 \]

Deformed Nuclei

\[ ^{16}O, \text{SIII, volume pairing, } \beta = -0.79 \]
PNP within DFT

Exact versus Approximate DFT

In the ideal case when the functional $E_N^{\rho}[\rho, \bar{\rho}]$ is exactly equivalent to an expectation value of a given Hamiltonian $H$ all residues from the poles $z_k > z_0$ are strictly zero and the energy is defined only by the residue of the zero pole $z_0 = 0$.

**Kinetic energy term** as well as all linear terms in the energy functional correspond to a power $a = 1$. Then all residues of $z_k > z_0$ will be zero since always one has $v_k \geq 1$.

**Coulomb energy** is a quadratic term, $a = 2$.
- The residue contribution of $z_k > z_0$ is zero assuming one treats the exchange term exactly – the residue from the direct coulomb term exactly cancels with the residue of the exchange term.
- If one uses Slater approximation for the exchange term such a cancelation does not exist anymore.

\[
\begin{align*}
\text{ph and pp contributions} \\
\text{ph channel:} \\
t_0 \frac{1}{4} (1 - x_0) \rho_n^2 + \frac{1}{4} (1 - x_0) \frac{u_k^2 v_k^2 z_k^2}{z_k^{N+1} (u_k^2 + v_k^2 z_k^2)^2} \\
\text{pp-channel:} \\
t_0 \frac{1}{4} (1 - x_0) \bar{\rho}_n^2 - \frac{1}{4} (1 - x_0) \frac{u_k^2 v_k^2 z_k^2}{z_k^{N+1} (u_k^2 + v_k^2 z_k^2)^2}
\end{align*}
\]

their sum cancels the pole contribution:

\[
\begin{align*}
\frac{1}{4} (1 - x_0) (\rho_n^2 + \bar{\rho}_n^2) & \rightarrow \frac{1}{4} (1 - x_0) \frac{u_k^2 v_k^2 z_k^2}{z_k^{N+1} (u_k^2 + v_k^2 z_k^2)^2}
\end{align*}
\]

In the case of Skyrme forces for which contact pairing forces are used instead the original Skyrme force, one will see nonzero contributions from the poles $z_k > z_0$ coming from both ph as well as pp terms.
PNP within DFT

Energy Sum Rule

\[ \tilde{E}(\eta) = \sum_{N} |b_{N}|^{2}E^{N}(\eta) \neq E_{HFB} \]

\[ \tilde{E}(\eta = 0) = E_{HFB} \]

\[ \tilde{E}(\eta = 0) = \sum_{N} |b_{N}|^{2}E^{N} = \int d\varphi \sum_{N} e^{-\nu N} \mathcal{I}(\varphi) E[\rho(\varphi), \tilde{\rho}(\varphi)] = E[\rho(0), \tilde{\rho}(0)] = E_{HFB} \]
Deformation Energy Calculations

- $E(\beta)$ (MeV)
- Deformation $\beta$

PNP within DFT

Deformation Energy Calculations

- $E_{PNC}$, $\beta$, SIII, vol. pairing
- E(PAV)
- Dynamical poles
- Lowest $d_{5/2}$ poles included
- Lowest $d_{5/2}$ poles excluded
- E(VAP)
- Lowest $d_{5/2}$ poles included
- Lowest $d_{5/2}$ poles excluded

- Neutron poles $z_k$

$^{16}$O, SIII, volume pairing

Theoretical Description of the Nuclear Large Amplitude Collective Motion, Oak Ridge, March 30-31, 2005
Deformation Energy Calculations

PNP within DFT

Theoretical Description of the Nuclear Large Amplitude Collective Motion, Oak Ridge, March 30-31, 2005
PNP Skyrme HFB Method

Conclusions

When no singularity exists on the unit circle

- LN method should be avoided
- PLN is a good for open shell nuclei
- PLN is wrong for closed shell nuclei
- One should try to correct PLN

\[ \text{One should use PLN instead} \]
\[ \text{Error is less than 250 KeV} \]
\[ \text{Error could be more than 1 MeV} \]

- Projecting from neighboring nuclei

All singularities cancel if EDF is exact

For an approximate functional:

- Shift Invariance is broken
- Energy Sum rule is not satisfied
- Density dependence is not analytical
- Instability in VAP

\[ \text{Locally it is satisfied} \]
\[ \text{Satisfied on the unit circle only} \]
\[ \text{Valid even for Gogny forces} \]
\[ \text{No solution at the moment} \]

PNP versus DFT