Density Functional Theory and Symmetry Restoration in Nuclei

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  - Energy Sum Rule
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Hohenberg-Kohn Theorem

Phys.Rev. 136 (1964) B846

The non-generate ground-state energy of a system of identical fermions is a unique functional of the local density which attains its minimal value, the ground-state energy of the system, when the density has its correct ground-state value.

N-representability

Gilbert, Phys.Rev. 2111 (1975) B12

$$\rho(\mathbf{r}) = N \int |\Psi(\mathbf{r}, \mathbf{r_2}, \mathbf{r_3}, ..., \mathbf{r_N})|^2 d\mathbf{r_2} d\mathbf{r_3} ... d\mathbf{r_N} \Longleftrightarrow$$

1) $\rho(\mathbf{r}) \geq 0$ everywhere in R^3
2) $\rho(\mathbf{r})^{1/2} \in L^2(R^3)$, i.e., $\int d\mathbf{r} \rho(\mathbf{r}) = N$
3) $\rho(\mathbf{r})$ continuously differentiable in R^3

$$H\Psi_0 = E_0 \Psi_0$$

$$\rho_0(\mathbf{r}) = N \int |\Psi_0(\mathbf{r}, \mathbf{r_2}, \mathbf{r_3}, ..., \mathbf{r_N})|^2 d\mathbf{r_2} d\mathbf{r_3} ... d\mathbf{r_N} \Longleftrightarrow$$

$$E[\rho] \geq E[\rho_0] = E_0$$

$$\frac{\delta E[\rho]}{\delta \rho(\mathbf{r})} - \lambda = 0$$

$$\int \rho(\mathbf{r}) d\mathbf{r} = N$$

$$\Psi \Longrightarrow \Psi[\rho] \quad \Rightarrow \quad E[\rho] = \frac{\langle \Psi[\rho] | \hat{H} | \Psi[\rho] \rangle}{\langle \Psi[\rho] | \Psi[\rho] \rangle}$$

Kohn-Sham Theory

Phys.Rev. 140 (1965) A1133

$$E[\rho] = T[\rho] + V[\rho] \qquad \frac{\delta T[\rho]}{\delta \rho(\mathbf{r})} + \frac{\delta V[\rho]}{\delta \rho(\mathbf{r})} = \lambda \qquad \int \rho(\mathbf{r}) d\mathbf{r} = N$$

$$\rho(r) = \sum_i^N |\phi_i(r)|^2$$

Harriman, J.E, Phys.Rev. 680 (1981) A24

$$\tau(r) = \sum_i^N |\nabla \phi_i(r)|^2 , \quad \tilde{T}[\rho] = \frac{\hbar^2}{2m} \int \tau(\mathbf{r}) d\mathbf{r} , \quad E[\rho] = \tilde{T}[\rho] + \tilde{V}[\rho] , \quad \tilde{V}[\rho] = V[\rho] + T[\rho] - \tilde{T}[\rho]$$

$$\left[-\frac{\hbar^2}{2m} \nabla^2 + U(\mathbf{r}, [\rho]) \right] \phi_i(\mathbf{r}) = e_i \phi_i(\mathbf{r}) , \qquad U(\mathbf{r}, [\rho]) = \frac{\delta \tilde{V}[\rho]}{\delta \rho(\mathbf{r})}$$

No idea about the many-body wave function of the system

No clear physical meaning of Kohn-Sham single-particle functions and energies

Widely used in atomic, molecular and condensed matter physics

HFB Method

Hamiltonian

$$H = \sum_{n_1 n_2} e_{n_1 n_2} \, c^\dagger_{n_1} c_{n_2} + \frac{1}{4} \sum_{n_1 n_2 n_3 n_4} \overline{v}_{n_1 n_2 n_3 n_4} \, c^\dagger_{n_1} c^\dagger_{n_2} c_{n_4} c_{n_3},$$

$$\overline{v}_{n_1 n_2 n_3 n_4} = \langle n_1 n_2 | V | n_3 n_4 - n_4 n_3 \rangle, \qquad c_n | - \rangle = 0.$$

Bogoliubov Transformation

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

$$\alpha_k | \Phi \rangle = 0, \qquad \hat{N} | \Phi \rangle \neq N | \Phi \rangle$$

$$\rho_{n'n} = \frac{\langle \Phi | c^\dagger_n c_{n'} | \Phi \rangle}{\langle \Phi | \Phi \rangle}, \quad \tilde{\rho}_{n'n} = \frac{\langle \Phi | s^*_{\bar{n}} c_{\bar{n}} c_{n'} | \Phi \rangle}{\langle \Phi | \Phi \rangle},$$

$$\hat{T} \phi_n(\mathbf{r}, \sigma) = s_n \phi_{\bar{n}}(\mathbf{r}, \sigma), \quad s_n s^*_n = 1, \quad s_{\bar{n}} = -s_n$$

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

HFB Equations

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

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

HFB Method

Particle Number Projection After Variation (PAV)

HFB Energy

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

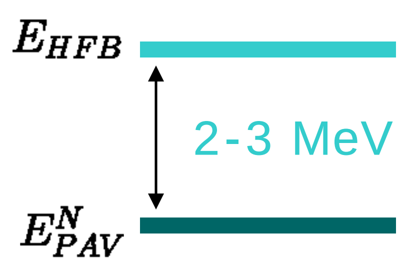
Particle Number Projection

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

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

PAV Energy

$$E^N_{PAV} = \frac{\langle \Psi^N | H | \Psi^N \rangle}{\langle \Psi^N | \Psi^N \rangle} = \frac{\langle \Phi | H P^N | \Phi \rangle}{\langle \Phi | P^N | \Phi \rangle}$$



HFB Method

Particle Number Projection - Variation After Projection (VAP)

PNP HFB Energy

$$E^N[\rho,\tilde\rho] = \frac{\langle\Phi|HP^N|\Phi\rangle}{\langle\Phi|P^N|\Phi\rangle} = \frac{\int d\phi\langle\Phi|He^{i\phi(\hat N-N)}|\Phi\rangle}{\int d\phi\langle\Phi|e^{i\phi(\hat N-N)}|\Phi\rangle}$$

PNP HFB (VAP)

$$\begin{pmatrix} \varepsilon^N+\Gamma^N+\Lambda^N & \Delta^N \\ -(\Delta^N)^* & -(\varepsilon^N+\Gamma^N+\Lambda^N)^* \end{pmatrix}\begin{pmatrix} U \\ V\end{pmatrix}_k = E_k^N\begin{pmatrix} U \\ V\end{pmatrix}_k$$

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

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

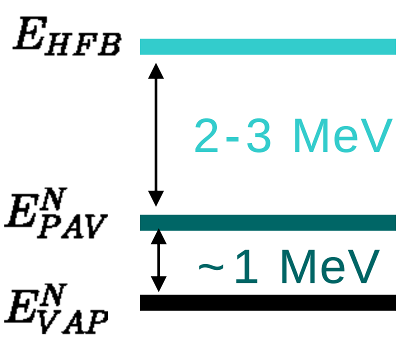
$$\Lambda^N = -\frac{1}{4}\int d\phi\; y(\phi)\left(Y(\phi)\mathrm{Tr}[\Delta(\phi)\overline{\kappa}^*(\phi)] - 4ie^{-i\phi}\sin\phi\; C(\phi)\Delta(\phi)\overline{\kappa}^*(\phi)\right) + h.c.$$

$$\Delta^N = \frac{1}{2}\int d\phi\; y(\phi)e^{-2i\phi}C(\phi)\,\Delta(\phi) - (..)^T,\quad \Gamma_{n_1n_3}(\phi) = \sum_{n_2n_4}\overline{v}_{n_1n_2n_3n_4}\rho_{n_4n_2}(\phi),$$

$$\Delta_{n_1n_2}(\phi) = \frac{1}{2}\sum_{n_3n_4}\overline{v}_{n_1n_2n_3n_4}\kappa_{n_3n_4}(\phi),\quad \overline{\Delta}^*_{n_3n_4}(\phi) = \frac{1}{2}\sum_{n_1n_2}\overline{\kappa}^*_{n_1n_2}(\phi)\overline{v}_{n_1n_2n_3n_4},$$

$$\begin{aligned}\rho(\phi) &= C(\phi)\rho \quad \kappa(\phi) = (\phi)\kappa = \kappa C^T(\phi)\\ \overline{\kappa}(\phi) &= e^{2i\phi}\kappa C^*(\phi) = e^{2i\phi}C^\dagger(\phi)\kappa\\ C(\phi) &= e^{2i\phi}\left(1+\rho(e^{2i\phi}-1)\right)^{-1},\end{aligned}$$

$$x(\phi) = \frac{1}{2\pi}\frac{e^{-i\phi N}\det(e^{i\phi}I)}{\sqrt{\det C(\phi)}},\quad y(\phi) = \frac{x(\phi)}{\int d\phi'\,x(\phi')},\quad \int d\phi\, y(\phi) = 1,$$



Skyrme HFB

- **SIII forces (density dependence as a tree body term)**
- **Both ph and pp interaction from the force**
- **Exact treatment of Coulomb terms**

Skyrme HFB Functional

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

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

$$\rho(\mathbf{r}\sigma,\mathbf{r}'\sigma') = \sum_{nn'} \rho_{nn'}\ \breve{\psi}^*_{n'}(\mathbf{r}',\sigma')\ \breve{\psi}_n(\mathbf{r},\sigma)$$

$$\tilde{\rho}(\mathbf{r}\sigma,\mathbf{r}'\sigma') = \sum_{nn'} \tilde{\rho}_{nn'}\ \breve{\psi}^*_{n'}(\mathbf{r}',\sigma')\ \breve{\psi}_n(\mathbf{r},\sigma)$$

Skyrme HFB Equations

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

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

Skyrme HFB as DFT

Main Problem

HFB

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

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

PNP HFB

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

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

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

The expectation value of the Hamiltonian is approximated as a density functional while keeping at the same time the HFB framework

'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

Energy Functional

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

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

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

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

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

Canonical Representation

Unprojected density $\rho_n = v_n^2,\quad \tilde{\rho}_n = u_n v_n \qquad \mathcal{I}(\varphi) = \prod_n\;(u_n^2 + v_n^2\; e^{2\imath\varphi}).$

'Mixed' density $\rho_n(\varphi) = \dfrac{v_n^2 e^{2\imath\varphi}}{u_n^2 + v_n^2\; e^{2\imath\varphi}}\;,\quad \tilde{\rho}_n(\varphi) = \dfrac{u_n v_n e^{\imath\varphi}}{u_n^2 + v_n^2\; e^{2\imath\varphi}}$

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

PNP HFB Equations

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

$$\begin{aligned} h^N &= \int d\phi y(\phi) Y(\phi) E(\phi) + \int d\phi y(\phi) e^{-2i\phi}\, C(\phi) h(\phi) C(\phi) \\ &- \left[\int d\phi y(\phi) 2ie^{-i\phi} sin(\phi) \tilde{\rho}(\phi) \tilde{h}(\phi) C(\phi) + h.c. \right], \\ \tilde{h}^N &= \int d\phi y(\phi) e^{-i\phi} \left(\tilde{h}(\phi) C(\phi) + (...)^T \right) \end{aligned}$$

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

Canonical Representation

$$\rho_n = v_n^2, \quad \tilde{\rho}_n = u_n v_n \qquad \rho_n(\varphi) = \frac{v_n^2 e^{2i\varphi}}{u_n^2 + v_n^2\, e^{2i\varphi}}, \quad \tilde{\rho}_n(\varphi) = \frac{u_n v_n e^{i\varphi}}{u_n^2 + v_n^2\, e^{2i\varphi}}$$

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

$$Y_\mu(\phi) = ie^{-i\phi} \sin\phi\, C_\mu(\phi) - \sum_{l'=0}^{L-1} y(\phi_{l'})\, ie^{-i\phi_{l'}} \sin\phi_{l'}\, C_\mu(\phi_{l'_\tau})$$

Grid Points

$$P^N = \frac{1}{2\pi} \int d\phi\, e^{i\phi(\hat{N}-N)} \Longrightarrow P^N = \frac{1}{L} \sum_{l=1}^{L} e^{i\phi_l(\hat{N}-N)}, \quad \phi_l = \frac{2\pi}{L}(l-1)$$

PNP Skyrme HFB Method

Problems: Stability

Slow (even unstable) procedure

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

$$Tr\rho = \bar{N}, \quad \rho = V^* V^T$$

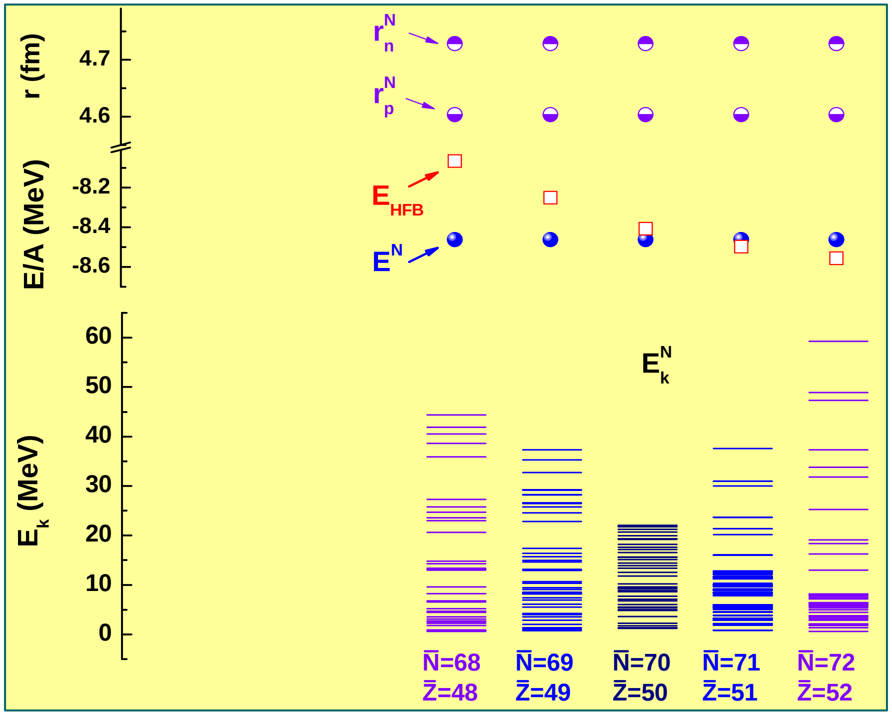
Stable procedure

$$\begin{pmatrix} h^N - \mu & \tilde{h}^N \\ \tilde{h}^N & -(h^N - \mu) \end{pmatrix} \begin{pmatrix} U \\ V \end{pmatrix}_k = E_k^N \begin{pmatrix} U \\ V \end{pmatrix}_k$$

$$Tr\rho = \bar{N}, \quad \rho = V^* V^T$$

μ is zero when the PNP solution is found

$$Tr\rho^N = N, \quad \rho^N = \int d\phi\, y(\phi) C(\phi)) \rho$$

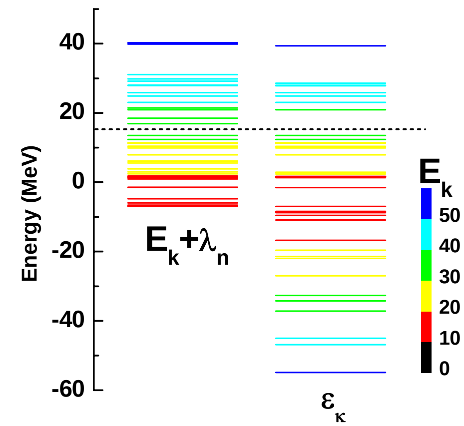


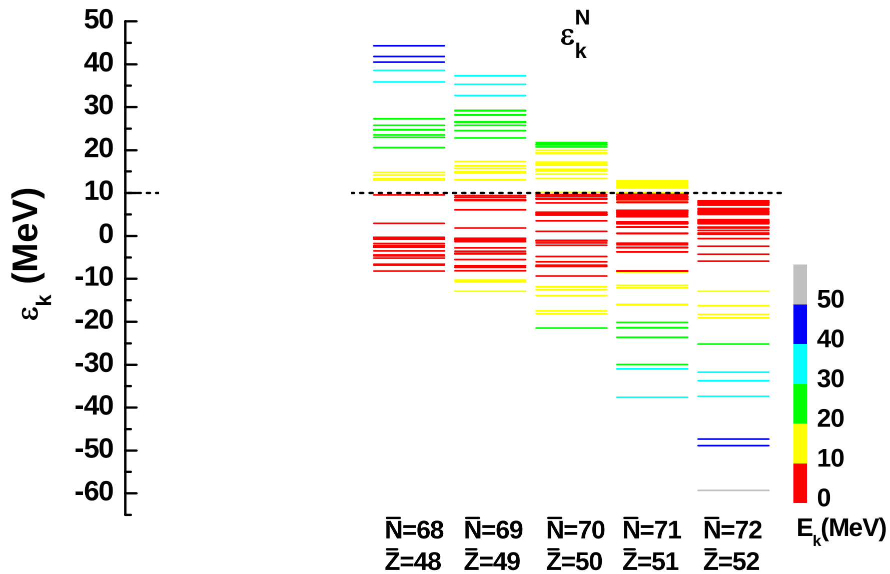
PNP Skyrme HFB Method

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 $\varphi = 0$

$$\tilde{E}_n = \begin{pmatrix} U \\ V \end{pmatrix}_n^\dagger \begin{pmatrix} h - \lambda & \tilde{h} \\ \tilde{h} & -h + \lambda \end{pmatrix} \begin{pmatrix} U \\ V \end{pmatrix}_n$$

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 $\epsilon_{\rm cut}$ reproduces the experimental value 1.245 MeV for the nucleus ^{120}Sn.

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

$$V_1 = \begin{cases} 0 \text{ voulme pairing} \\ 1 \text{ surface pairing} \end{cases}$$

$$\gamma = 1, \quad \rho_0 = 0.16 \text{ fm}^{-3}$$

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.

PNP Skyrme HFB Method

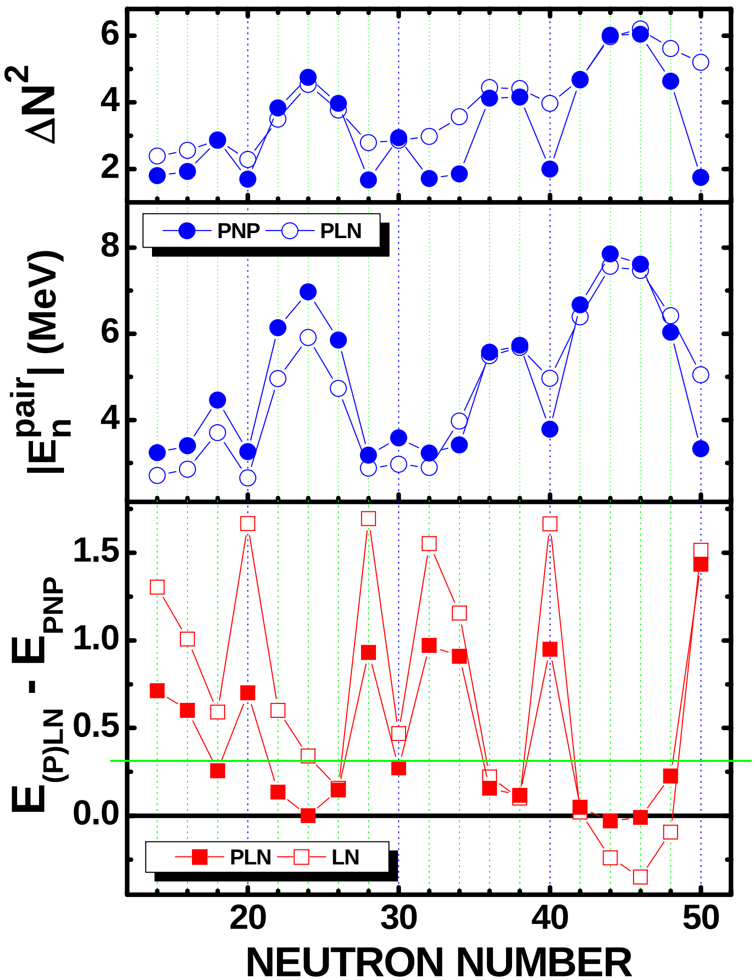
Ca Chain Calculations

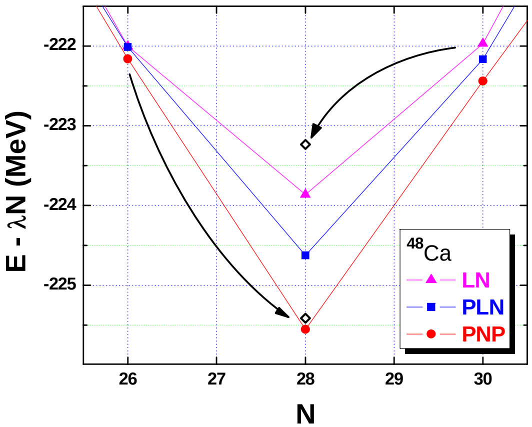
- **SLY4 + mixed delta pairing forces**
- **HFB within 20 major HO shells**
- **Complete Ca chain**
- **Comparison:**
  - **HFB+LN results (LN)**
  - **PAV HFB+LN results (PLN)**
  - **VAP PNP HFB results (PNP)**
- **PLN pairing strength fitted to Δ_n @ ^{120}Sn**
- **PNP pairing strength to PLN E_{tot}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

- **With L=11 gauge-angle points the code is just 11 times slower**

PNP Skyrme HFB Method

Some Results





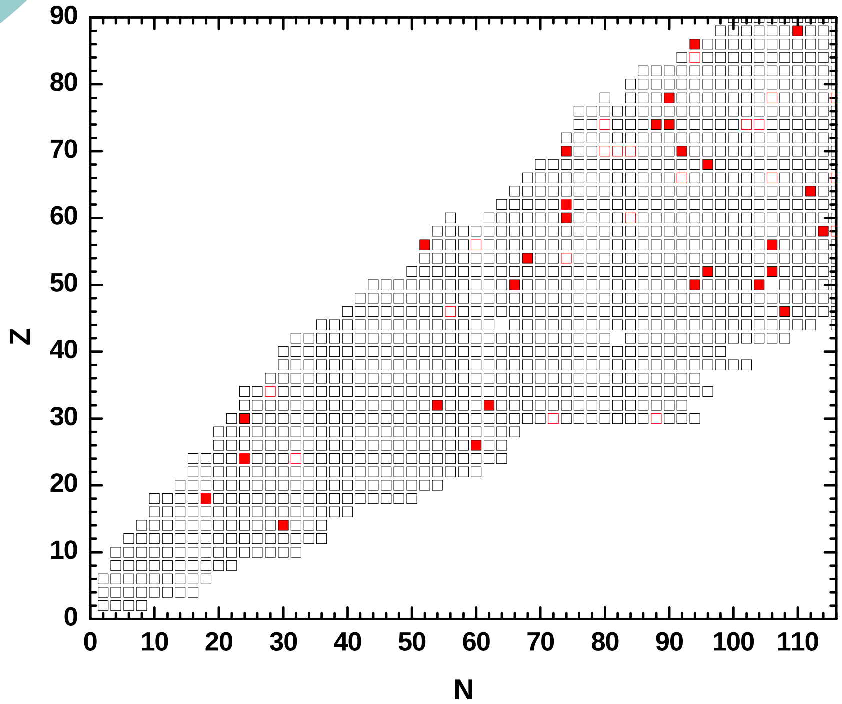
- LN method should be avoided
  - One should use PLN instead
- PLN is a good approximation for open shell nuclei
  - total energy differences are less than 250 KeV
- PLN is wrong for closed shell nuclei
  - total energy differences could be more than 1 MeV
- One should try to correct PLN by projecting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

PNP within DFT

Well Known Singularity

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

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



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

Exact Relations

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

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

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

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

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

Shift Invariance

$$\underbrace{e^{\eta(\hat{N}-N)}}_{\hat{S}_\eta}|\Psi_N\rangle = |\Psi_N\rangle, \quad \hat{N}|\Psi_N\rangle = N|\Psi_N\rangle \quad E^N = \frac{\langle\Phi|\hat{H}|\Psi_N\rangle}{\langle\Phi|\Psi_N\rangle} = \frac{\langle\Phi|\hat{H}\hat{S}_\eta|\Psi_N\rangle}{\langle\Phi|\hat{S}_\eta|\Psi_N\rangle}$$

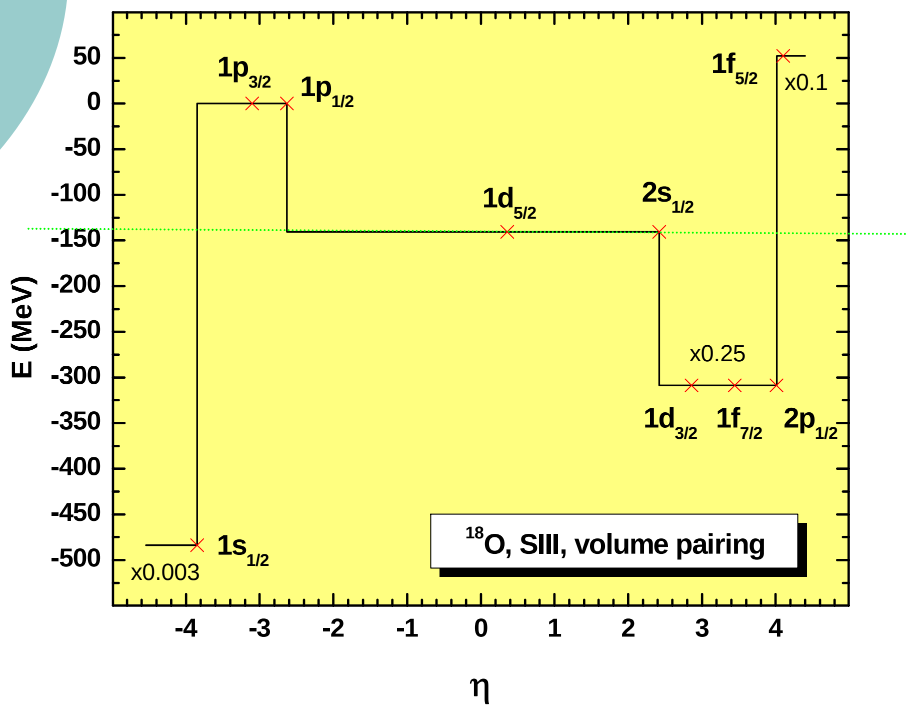
Energy Sum Rule

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

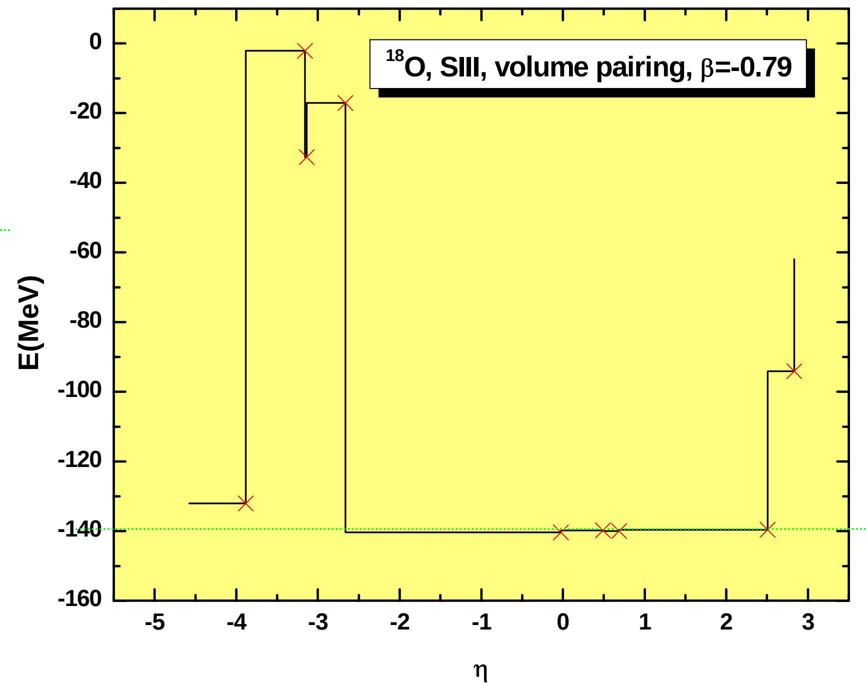
PNP within DFT

Broken Shift Invariance

Spherical Nuclei



Deformed Nuclei



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PNP within DFT

PNP Energy

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

$$\mathcal{I}(\varphi) \;=\; \langle\Phi(0)|\Phi(\varphi)\rangle = \prod_n \;(u_n^2 + v_n^2\; e^{2\imath\varphi})$$

$$\rho_n(\varphi) = \frac{v_n^2 e^{2\imath\varphi}}{u_n^2 + v_n^2\; e^{2\imath\varphi}}\;, \quad \tilde\rho_n(\varphi) = \frac{u_n v_n e^{\imath\varphi}}{u_n^2 + v_n^2\; e^{2\imath\varphi}}$$

New complex variable

$$z = e^{\imath\varphi}, \quad d\varphi = \tfrac{dz}{\imath z}, \quad C_1(|z|=1) \quad \rho_n(z) = \frac{v_n^2 z^2}{u_n^2 + v_n^2\; z^2}\;, \quad \tilde\rho_n(z) = \frac{u_n v_n\; z}{u_n^2 + v_n^2\; z^2}$$

$$\mathcal{N}_N \equiv \int d\varphi\, e^{-\imath\varphi N}\mathcal{I}(\varphi)\; E[\rho(\varphi),\tilde\rho(\varphi)] = -\imath \oint \frac{dz}{z^{N+1}} \prod_n \;(u_n^2 + v_n^2\; z^2) E[\rho(z),\tilde\rho(z)]$$

$$\mathcal{D}_N \equiv \int d\varphi\; e^{-\imath\varphi N}\; \mathcal{I}(\varphi) = \oint \frac{dz}{z^{N+1}} \prod_n \;(u_n^2 + v_n^2\; z^2)$$

Cauchy's residue theorem

$$\oint_C dz f(z) = 2\pi\imath \sum_k Rez[f(z_k)] \qquad z_k = \pm\imath\; |u_k/v_k|$$

$$\mathcal{N}_N = 2\pi\imath \sum_{|z_k|\le 1} Rez\left[\frac{1}{z_k^{N+1}} \prod_n \;(u_n^2 + v_n^2\; z_k^2) E[z_k]\right]$$

$$\mathcal{D}_N = 2\pi\imath\; Rez\left[\frac{1}{z_0^{N+1}} \prod_n \;(u_n^2 + v_n^2\; z_0^2)\right]$$

PNP within DFT

PNP Energy

$$E_N = E_N[z_0] + \Delta E_N \qquad z_0 = 0, \quad z_k = \pm\imath\,|u_k/v_k|$$

$$E_N[z_0] = \frac{Rez\left[\frac{1}{z_0^{N+1}}\prod_n (u_n^2 + v_n^2\ z_0^2)E[z_0]\right]}{Rez\left[\frac{1}{z_0^{N+1}}\prod_n (u_n^2 + v_n^2\ z_0^2)\right]} \qquad \Delta E_N = \frac{2\pi\imath}{\mathcal{D}_N}\sum_{0<|z_k|\le 1} Rez\left[\prod_n (u_n^2 + v_n^2\ z_k^2)\frac{E[z_k]}{z_k^{N+1}}\right]$$

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 ρ, p power of $\tilde\rho$
- ν_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 $j = 3/2$ ...

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

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

Shifted PNP Energy

$$\underbrace{e^{\eta(\hat N - N)}}_{\hat S_\eta}|\Psi_N\rangle$$

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

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

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

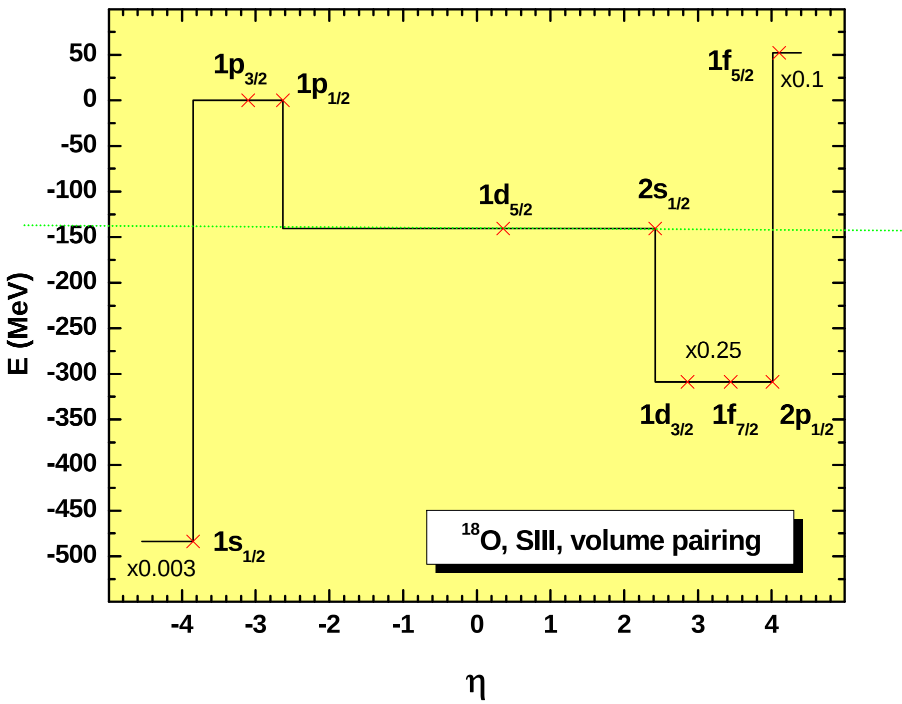
PNP within DFT

Local Shift Invariance

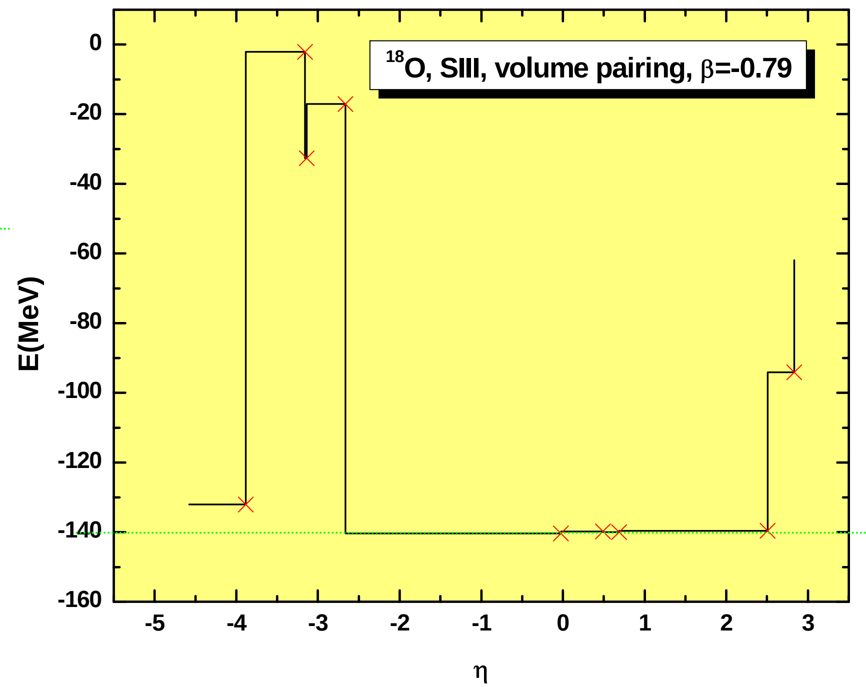
$$E_N(\eta) = E_N[z_0] + \Delta E_N(\eta) \qquad z_0 = 0, \quad z_k = \pm \imath \, |u_k/v_k| \Leftrightarrow u_k^2 = v_k^2 = \frac{1}{2}, \quad \varphi = \frac{\pi}{2}$$

$$E_N[z_0] = \frac{Rez\left[\frac{1}{z_0^{N+1}} \prod_n \left(u_n^2 + v_n^2\, z_0^2\right) E[z_0]\right]}{Rez\left[\frac{1}{z_0^{N+1}} \prod_n \left(u_n^2 + v_n^2\, z_0^2\right)\right]} \qquad \Delta E_N(\eta) = \sum_{|z_k| \le e^{-\eta}} \sum_a Rez\left[\frac{\left(u_k^2 + v_k^2\, z_k^2\right)^{\nu_k} f_a(z_k)}{z_k^{N+1}\left(u_k^2 + v_k^2\, z_k^2\right)^a}\right]$$

Spherical Nuclei



Deformed Nuclei



PNP within DFT

Exact versus Approximate DFT

In the ideal case when the functional $E^N[\rho, \tilde{\rho}]$ 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 $\nu_k \geq 1$.**

pp and ph contributions

ph channel:

$$\frac{t_0}{4}(1-x_0)\rho_n^2 \rightarrow \frac{t_0}{4}(1-x_0)\frac{v_k^4 z_k^4}{z_k^{N+1}(u_k^2 + v_k^2\, z_k^2)^2}$$

pp-channel:

$$\frac{t_0}{4}(1-x_0)\tilde{\rho}_n^2 \rightarrow \frac{t_0}{4}(1-x_0)\frac{u_k^2 v_k^2 z_k^2}{z_k^{N+1}(u_k^2 + v_k^2\, z_k^2)^2}$$

their sum cancels the pole contribution:

$$\frac{t_0}{4}(1-x_0)(\rho_n^2+\tilde{\rho}_n^2) \rightarrow \frac{t_0}{4}(1-x_0)\frac{v_k^2 z_k^2}{z_k^{N+1}(u_k^2 + v_k^2\, z_k^2)}$$

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.

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.**

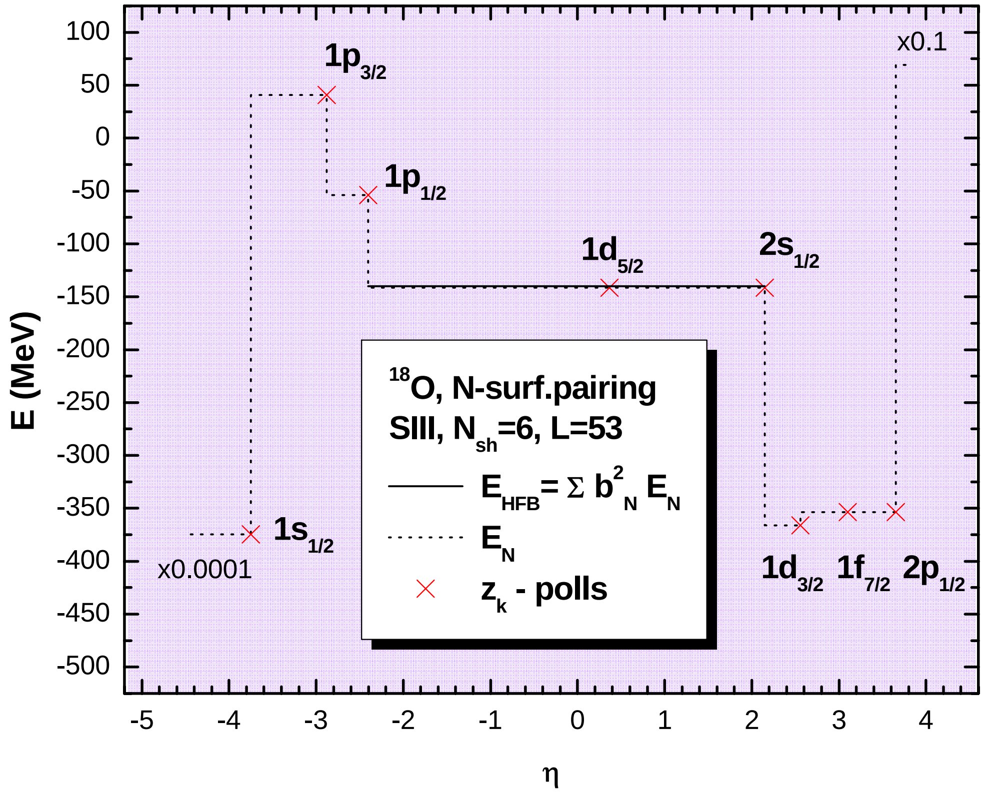
PNP within DFT

Energy Sum Rule

$$\tilde{E}(\eta) = \sum_N |b_N|^2 E^N(\eta) \neq E_{HFB}$$

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

$$\tilde{E}(\eta = 0) = \sum_N |b_N|^2 E^N \;=\; \int d\varphi \sum_N e^{-\imath\varphi N} \mathcal{I}(\varphi) E[\rho(\varphi), \tilde{\rho}(\varphi)] = E[\rho(0), \tilde{\rho}(0)] = E_{HFB}$$



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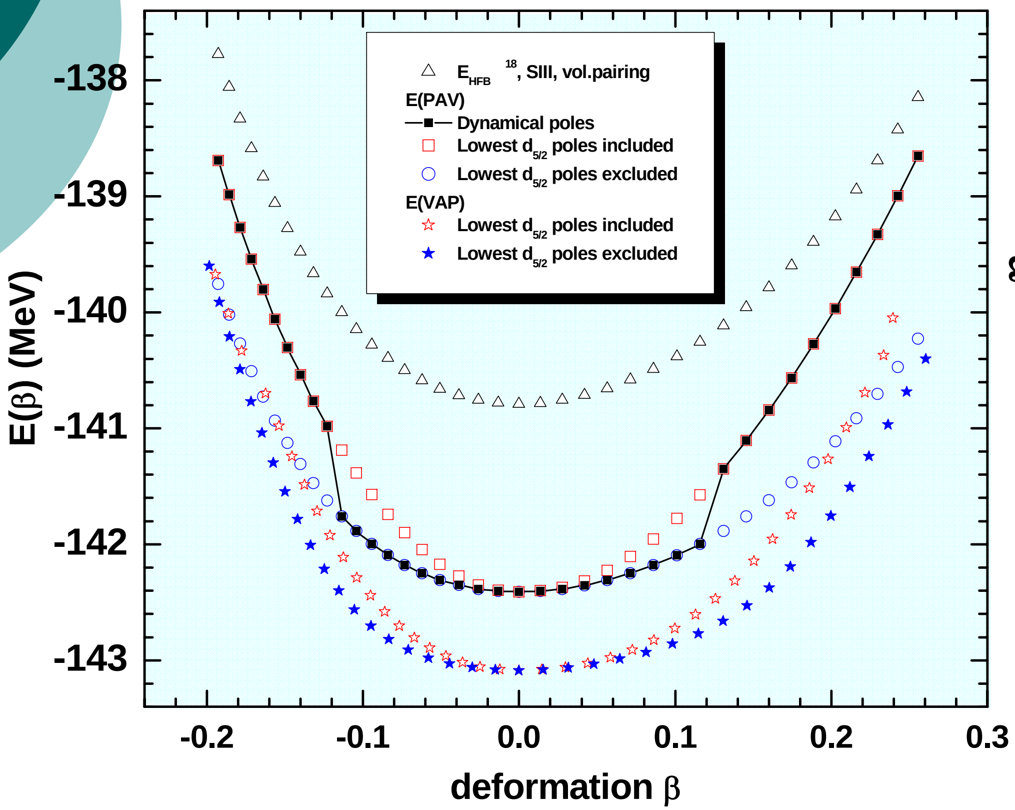
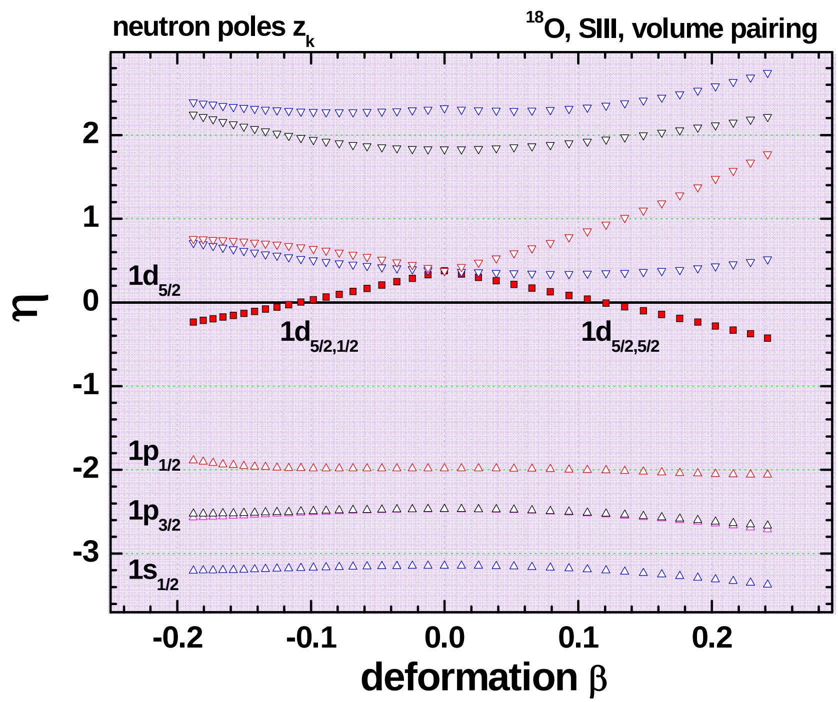
PNP within DFT

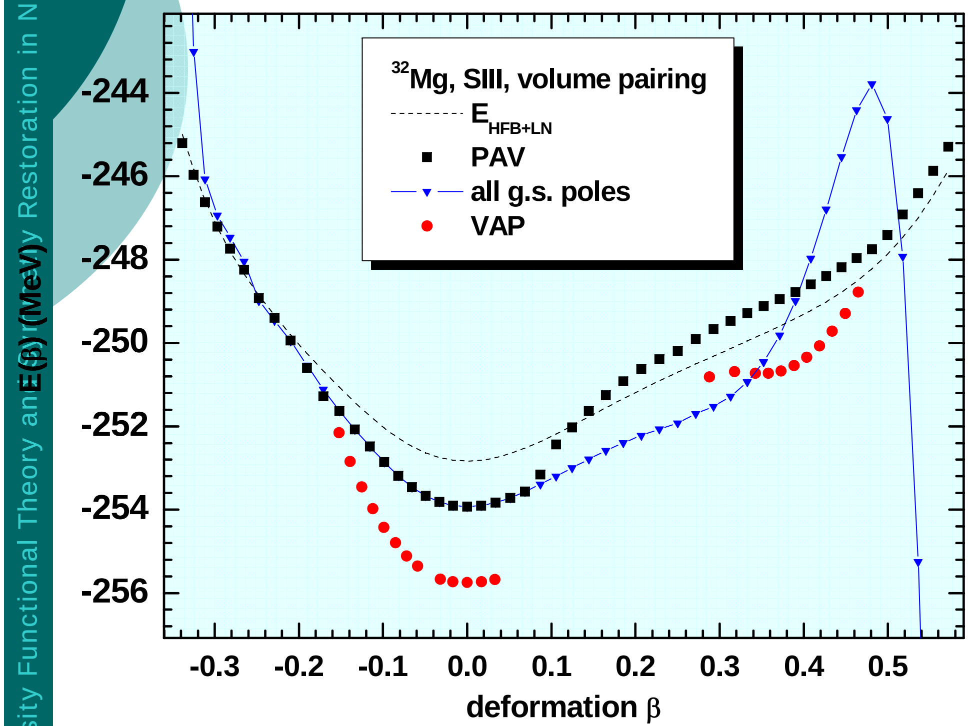
Deformation Energy Calculations

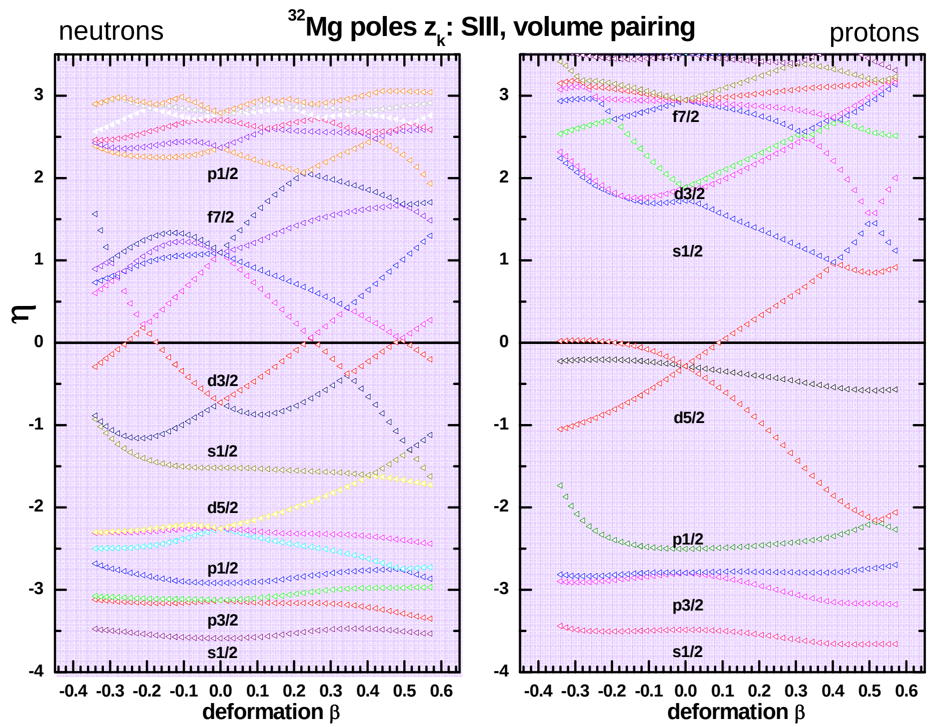




PNP within DFT

Deformation Energy Calculations





PNP Skyrme HFB Method

Conclusions

When no singularity exists on the unit circle

- **LN method should be avoided** – **One should use PLN instead**
- **PLN is a good for open shell nuclei** – **Error is less than 250 KeV**
- **PLN is wrong for closed shell nuclei** – **Error could be more than 1 MeV**
- **One should try to correct PLN** – **Projecting from neighboring nuclei**

PNP versus DFT

- **All singularities cancel if EDF is exact**

For an approximate functional:

- **Shift Invariance is broken** – **Locally it is satisfied**
- **Energy Sum rule is not satisfied** – **Satisfied on the unit circle only**
- **Density dependence is not analytical** – **Valid even for Gogny forces**
- **Instability in VAP** – **No solution at the moment**