Restoring Broken Symmetries within the nuclear EDF method: *Regularization of non-diagonal energy density functional kernels*

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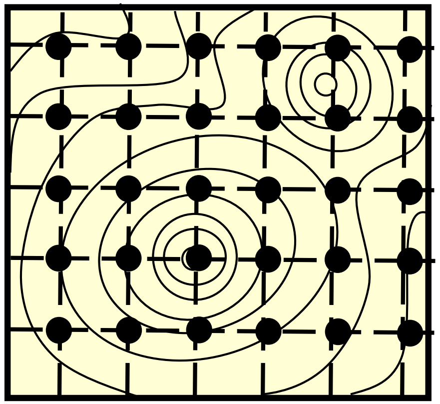
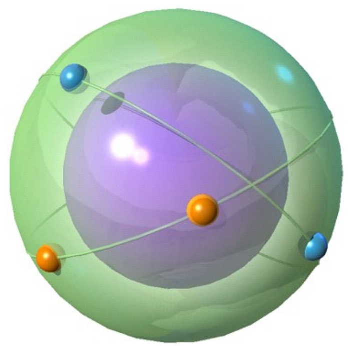
Outline of my talk

Multi- Ref. (MR)-GCM



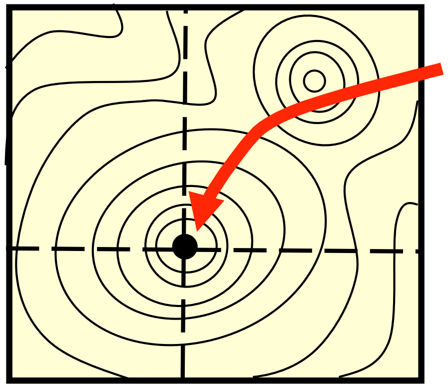
- Some recent discussion on symmetry breaking and Restoration in Energy Density Functional theory
  - ⇨ Hamiltonian vs EDF
  - ⇨ Self-interaction problem
  - ⇨ Regularization in EDF
  - ⇨ Density dependence of effective interaction ?
  - ⇨ Can we interpret the MR-EDF as a functional theory?

- Proposition of a different strategy to break and restore symmetry in EDF : The Symmetry-Conserving EDF concept
  - ⇨ Application to Particle number Restoration
  - ⇨ Examples of application of Projection before or After variation to light and medium mass nuclei



Configuration Mixing within Energy Density Functional

Single Reference (SR)-Mean-Field



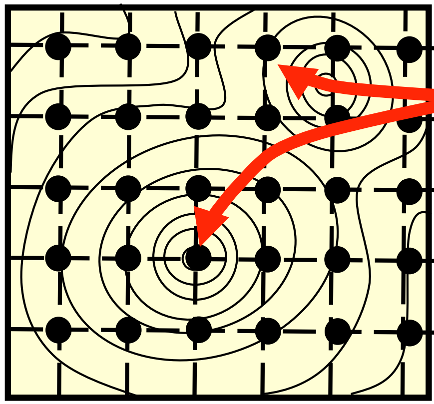
$$|\Phi\rangle = \Pi \alpha_k |0\rangle$$

(Skyrme, Gogny)

$$\langle \Phi(Q) | \hat{H} | \Phi(Q) \rangle$$

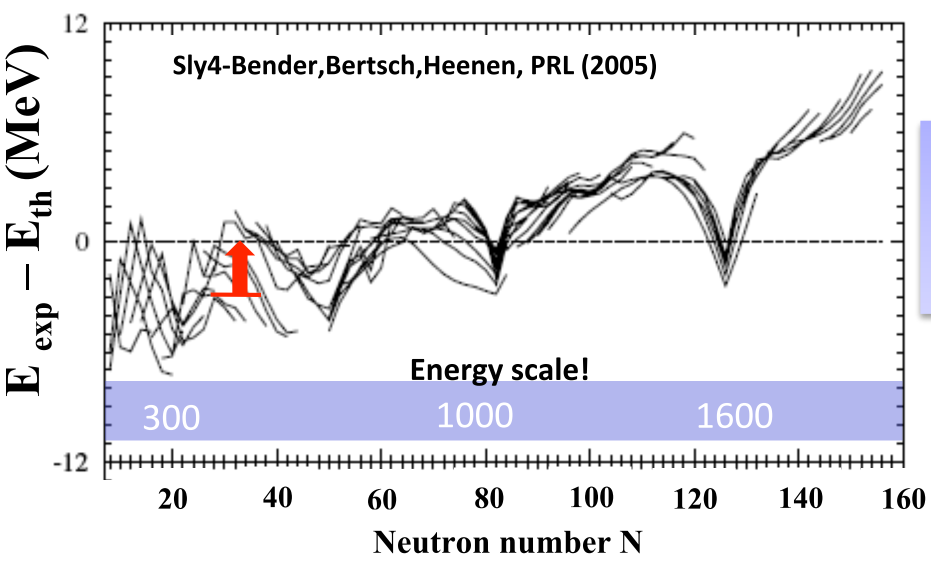
Multi- Ref. (MR)-GCM

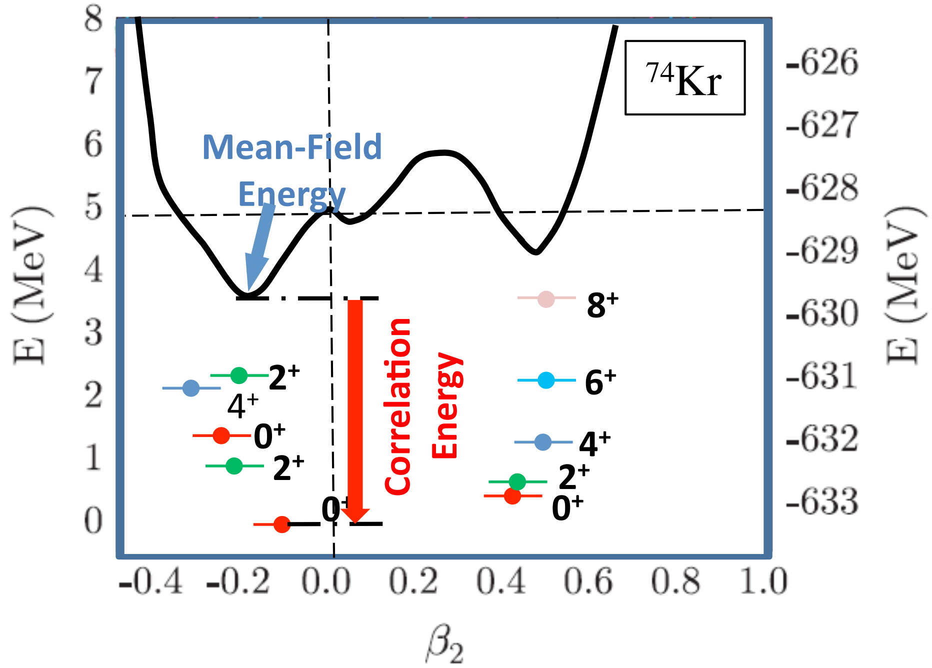
$$|\Psi\rangle = \int dQ f(Q) |\Phi(Q)\rangle$$



$$|\Phi(Q_i)\rangle$$

$$\langle \Psi | \hat{H} | \Psi \rangle$$



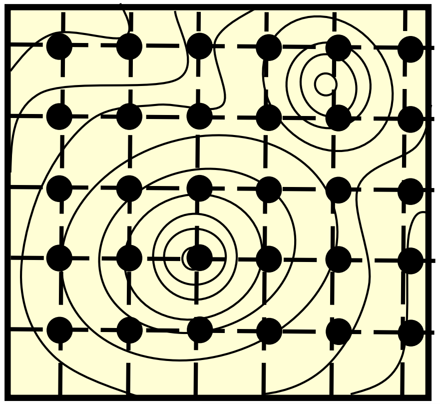


Bender et al, PRC74 (2006)

Inclusion of correlation through symmetry breaking:

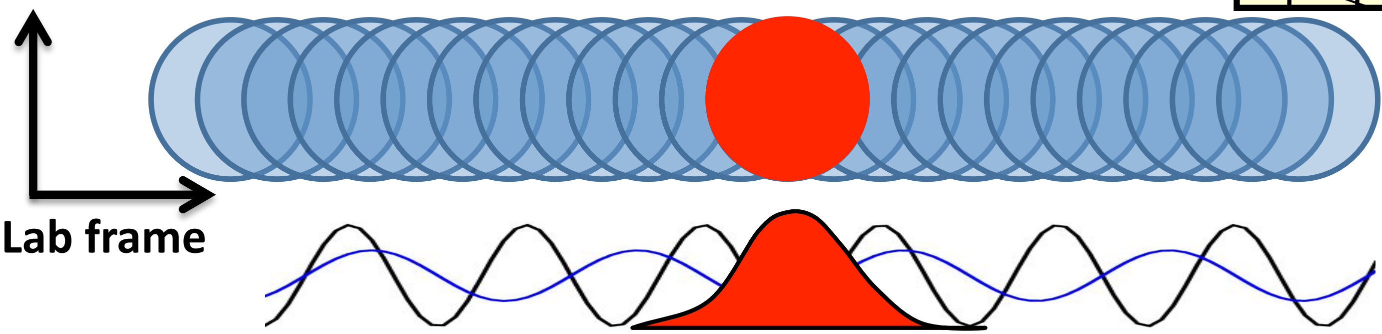
EDF breaks as much as possible symmetries
to incorporate correlations

Multi- Ref. (MR)-GCM



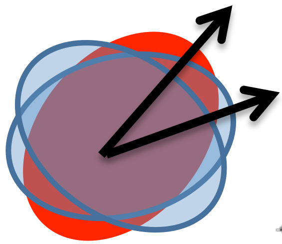
Few examples

- translational invariance ⇨ $[\hat{H}, \hat{P}_{\rm cm}] \neq 0$



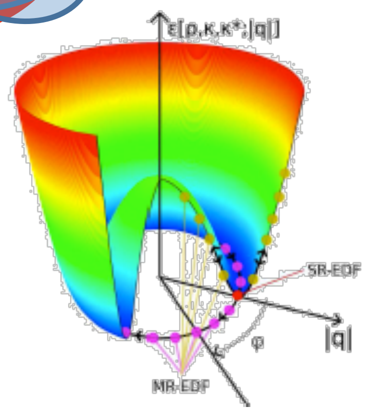
Surface Vibration

- Rotational invariance ⇨ $[\hat{H}, \hat{J}] \neq 0$



Quadrupole Correlation
-
Rotational Bands

- U(1) symmetry ⇨ $[\hat{H}, \hat{N}] \neq 0$



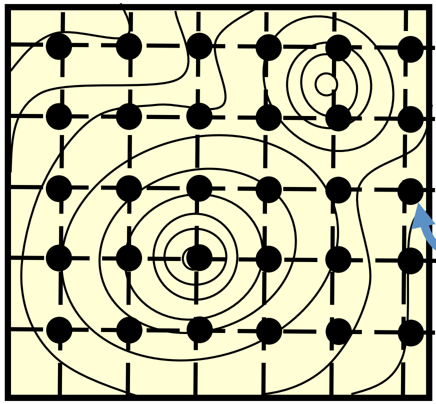
Pairing Correlations
-
Odd-even effects

In all cases: $|\Psi\rangle = \int dQ f(Q) \, |\Phi(Q)\rangle$

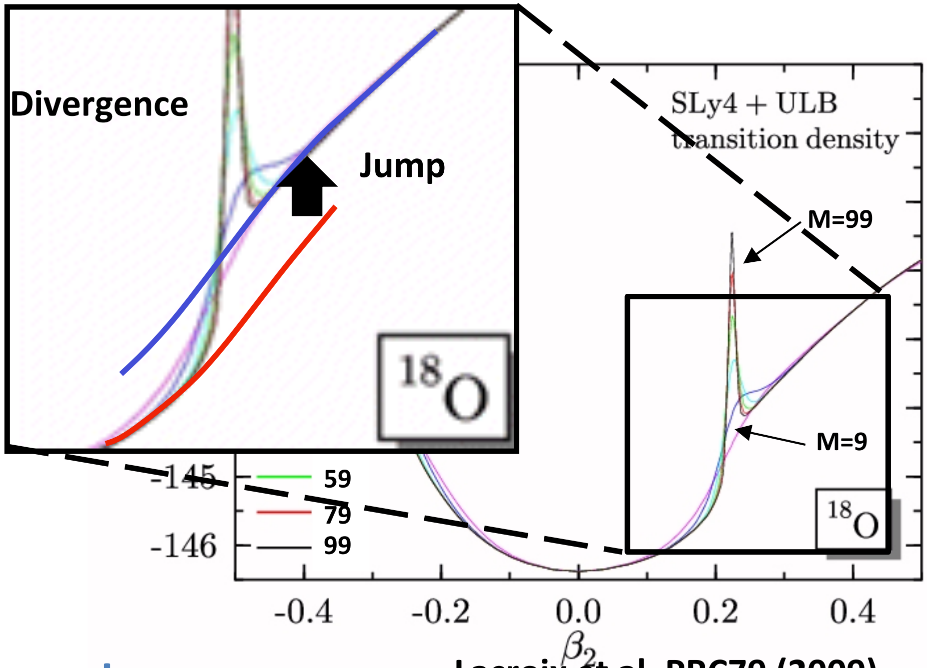
Ring and Schuck book (1980)

Application of conf. mixing in EDF
Needs to be regularized

Multi- Ref. (MR)-GCM



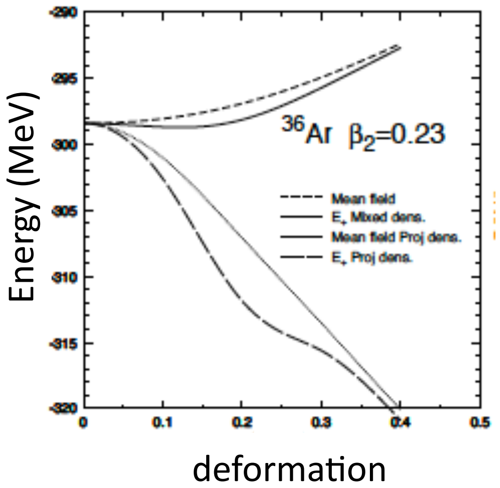
M: number of Mesh points



Only functional of ρ, ρ^2, ρ^3, ρ^4, ρ^5 could be used, not ρ^α !!

Lacroix et al, PRC79 (2009),
Bender et al, PRC79 (2009),
Duguet et al, PRC79 (2009)

What should be the density to be used in the effective interaction ?



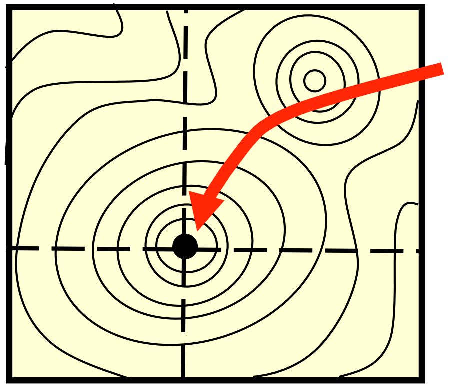
Taken from
L. M. Robledo, J. Phys. G 37 (2010)

The very notion of symmetry restoration in EDF needs to be clarified

T. Duguet and J. Sadoudi, J. Phys. G 37 (2010)

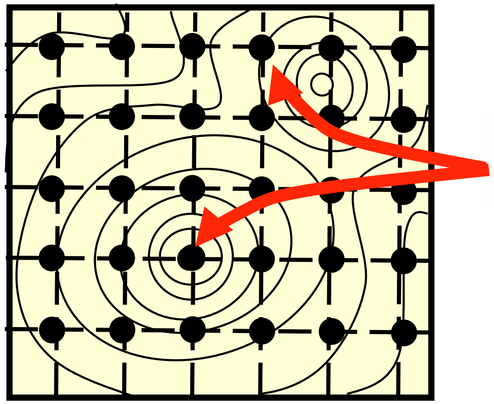
Multi-Reference: Generalities and difficulties

Single Reference (SV)



$$|\Phi\rangle = \Pi\alpha_k |0\rangle$$

Multi- Ref. (MR)



$$|\Phi(Q_i)\rangle$$

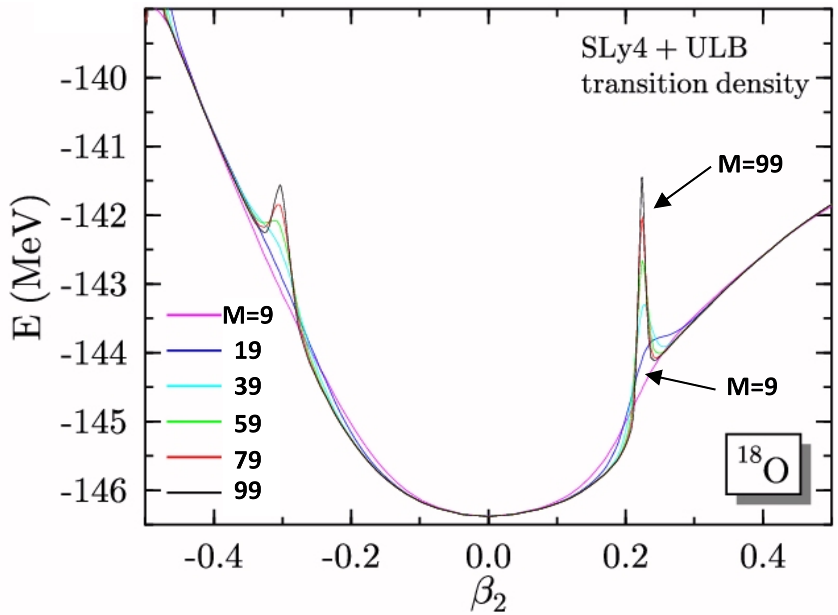
Example: Particle Number Restoration

$$|\Psi^N\rangle = \int_0^{2\pi} d\varphi \, \frac{e^{-i\varphi N}}{2\pi \, c_N} |\Phi[\varphi]\rangle$$

with $$|\Phi[\varphi]\rangle = e^{i\varphi \hat{N}} |\Phi_0\rangle$$

PNR (or PNP) on a mesh

$$\Rightarrow \sum_{k=1}^{M} \Delta\varphi \, \frac{e^{-i\varphi_k N}}{2\pi \, c_N} |\Phi[\varphi_k]\rangle$$



Bender, Duguet,
Int. J. Mod. Phys. E16 (2007)

Phenomenology of divergences in the PNP case

- Tajima et al, NPA542 (1992)

  ➡ Early warnings

- Anguiano et al, NPA 696 (2001)

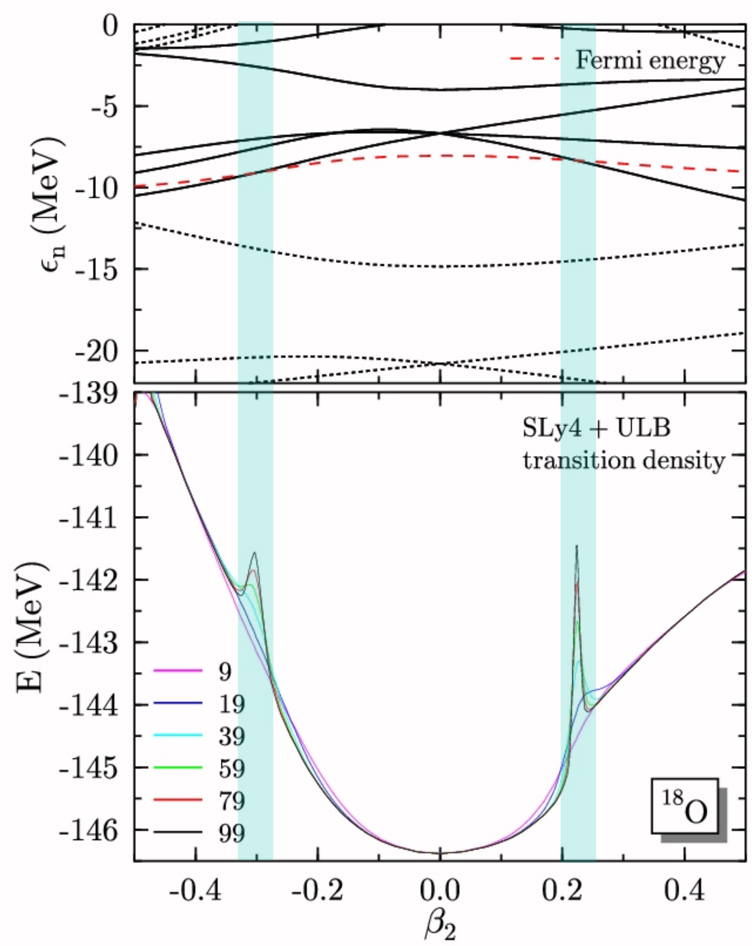
  ➡ Divergences occur when a level crosses the Fermi energy, with occupation 0.5 and φ=π/2 at this point $\langle \Phi_0 | \Phi[\varphi] \rangle = 0$

  ➡ The problem disappears if the same interaction (with exchange and coulomb treated properly) in the pp and ph channels.

  ➡ First indication of the role of Generalized Wick Theorem (GWT)

- Dobaczewski et al, *arXiv:0708.0441*

  ➡ Analysis in the complex plane for the PNP case



- Bender and Duguet, Int.J. Mod. Phys. E16 (2007)

  ➡ In the PNP case, by avoiding the use of GWT, one can cure the divergence problem even when different effective interaction are used in different channels.

Starting point: Effective Hamiltonian (Skyrme, Gogny,…)

$$\hat{H} = \sum_{ij} t_{ij}\, a_i^+ a_j + \frac{1}{4}\sum_{ijkl} \bar{v}_{ijkl}\, a_i^+ a_j^+ a_l a_k + \cdots \xrightarrow{\text{EDF}} \langle \Phi_0 | \hat{H} | \Phi_0 \rangle = (UNEDF)\langle \Phi_0 | \Phi_0 \rangle$$

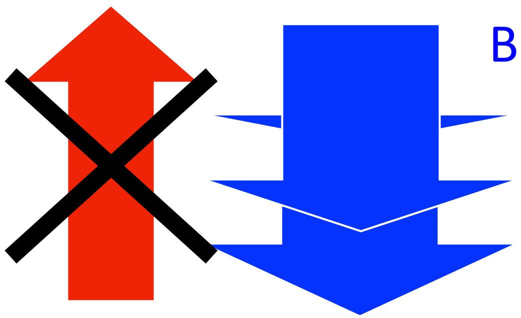
Effective Hamiltonian Case (Standard Wick Theorem)

$$\frac{\langle \Phi_0 | \hat{H} | \Phi_0 \rangle}{\langle \Phi_0 | \Phi_0 \rangle} = \sum_{ij} t_{ij}\, \rho_{ji}^{00} + \frac{1}{2}\sum_{ijkl} \bar{v}_{ijkl}\, \rho_{ki}^{00}\, \rho_{lj}^{00} + \frac{1}{4}\sum_{ijkl} \bar{v}_{ijkl}\, \kappa_{ij}^{00\,*}\, \kappa_{kl}^{00}$$

$$\equiv \mathcal{E}^H(\rho^{00}, \kappa^{00}, \kappa^{00\,*})$$

$$\rho_{ij}^{00} = \frac{\langle \Phi_0 | a_j^+ a_i | \Phi_0 \rangle}{\langle \Phi_0 | \Phi_0 \rangle}$$

$$\kappa_{ij}^{00} = \frac{\langle \Phi_0 | a_j a_i | \Phi_0 \rangle}{\langle \Phi_0 | \Phi_0 \rangle}$$



Breaking the link with the Hamiltonian

- Introduction of new terms ρ^γ
- Different interactions in ph and pp channels $\bar{v}^{\rho\rho} \neq \bar{v}^{\kappa\kappa}$
- Technical issues: coulomb, exchange…

Energy Density Functional Case

$$\mathcal{E}^{EDF}(\rho^{00}, \kappa^{00}, \kappa^{00\,*}) = \sum_{ij} t_{ij}\, \rho_{ji}^{00} + \frac{1}{2}\sum_{ijkl} \bar{v}_{ijkl}^{\rho\rho}\, \rho_{ki}^{00}\, \rho_{lj}^{00} + \frac{1}{4}\sum_{ijkl} \bar{v}_{ijkl}^{\kappa\kappa}\, \kappa_{ij}^{00\,*}\, \kappa_{kl}^{00}$$

Construction of EDF for configuration mixing:

the "nuclear physics strategy"

Starting point: Effective Hamiltonian (Skyrme, Gogny,…)

$$\hat{H} = \sum_{ij} t_{ij}\, a_i^+ a_j + \frac{1}{4}\sum_{ijkl} \bar{v}_{ijkl}\, a_i^+ a_j^+ a_l a_k + \cdots$$

EDF →

$$\langle \Phi_0 | \hat{H} | \Phi_1 \rangle = (UNEDF) \langle \Phi_0 | \Phi_1 \rangle$$

Effective Hamiltonian case

Single-R

Standard Wick Theorem

$$\mathcal{E}^{H}(\rho^{00}, \kappa^{00}, \kappa^{00\,*})$$

$$\rho_{ij}^{00} = \frac{\langle \Phi_0 | a_j^+ a_i | \Phi_0 \rangle}{\langle \Phi_0 | \Phi_0 \rangle} \;, \quad \kappa_{ij}^{00} = \frac{\langle \Phi_0 | a_j a_i | \Phi_0 \rangle}{\langle \Phi_0 | \Phi_0 \rangle}$$

Multi-R

Generalized Wick Theorem

$$\mathcal{E}^{H}(\rho^{01}, \kappa^{01}, \kappa^{10\,*})$$

$$\rho_{ij}^{01} = \frac{\langle \Phi_0 | a_j^+ a_i | \Phi_1 \rangle}{\langle \Phi_0 | \Phi_1 \rangle} \;, \quad \kappa_{ij}^{01} = \frac{\langle \Phi_0 | a_j a_i | \Phi_1 \rangle}{\langle \Phi_0 | \Phi_1 \rangle} \;, \ldots$$

Balian, Brezin, Nuovo Cimento 64 (1969)

EDF case

$$\mathcal{E}^{EDF}(\rho^{00}, \kappa^{00}, \kappa^{00\,*})$$

$$\rho_{ij}^{00} = \frac{\langle \Phi_0 | a_j^+ a_i | \Phi_0 \rangle}{\langle \Phi_0 | \Phi_0 \rangle} \;, \quad \kappa_{ij}^{00} = \frac{\langle \Phi_0 | a_j a_i | \Phi_0 \rangle}{\langle \Phi_0 | \Phi_0 \rangle}$$

$$\mathcal{E}^{EDF}(\rho^{01}, \kappa^{01}, \kappa^{01\,*})$$

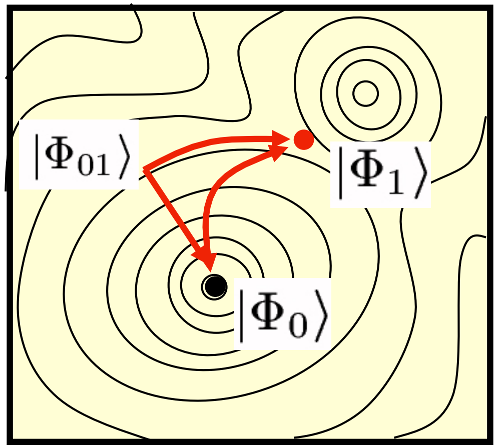
$$\rho_{ij}^{01} = \frac{\langle \Phi_0 | a_j^+ a_i | \Phi_1 \rangle}{\langle \Phi_0 | \Phi_1 \rangle} \;, \quad \kappa_{ij}^{01} = \frac{\langle \Phi_0 | a_j a_i | \Phi_1 \rangle}{\langle \Phi_0 | \Phi_1 \rangle} \;, \ldots$$

→ *Practical difficulties*

→ *Origin of divergences*

$$\rho^{\gamma}$$

Methods for connecting different quasi-particle vacua



Starting points:

Topology of reference state

$$|\Phi_0\rangle = \mathcal{C}_0 \prod \alpha_\nu |0\rangle$$

$$|\Phi_1\rangle = \mathcal{C}_1 \prod_\nu \beta_\nu |0\rangle$$

$$\alpha_\nu^+ = \sum_i (U_{i\nu}^0\, a_i^+ + V_{i\nu}^0\, a_i)$$

$$\beta_\nu^+ = \sum_i (U_{i\nu}^1\, a_i^+ + V_{i\nu}^1\, a_i)$$

$$\beta_\mu^+ = \sum_\nu (A_{\nu\mu}\, \alpha_\nu^+ + B_{\nu\mu}\, \alpha_\nu)$$

$$A = U^{0^+} U^1 + V^{0^+} V^1$$

$$B = V^{0^T} U^1 + U^{0^T} V^1$$

The Balian-Brezin (Thouless) strategy

Start from $|\Phi_1\rangle \propto e^{\mathcal{S}(\alpha,\alpha^+)}|\Phi_0\rangle$

$$\beta = e^{\mathcal{S}} \alpha e^{-\mathcal{S}}$$

valid for $\langle\Phi_0\,|\,\Phi_1\rangle \neq 0$

Work on the transformation

$$\frac{\langle\Phi_0|\hat{H}|\Phi_1\rangle}{\langle\Phi_0\,|\,\Phi_1\rangle} = \mathcal{E}^H(\rho^{01}, \kappa^{01}, \kappa^{10\,*})$$

$\langle\Phi_0\,|\,\Phi_1\rangle = 0$ → ***Donau PRC(1998), Dobaczewski PRC(2000)***

The Bloch-Messiah-Zumino Strategy

Work directly on A and B

$$A = D\bar{A}C \quad B = D^*\bar{B}C$$

$$\alpha \overset{D}{\rightarrow} \tilde{\alpha} \qquad \beta \overset{C}{\rightarrow} \tilde{\beta}$$

$$\bar{B}(p) = \begin{pmatrix} 0 & \bar{B}_{p\bar{p}} \\ \bar{B}_{\bar{p}p} & 0 \end{pmatrix} \qquad \bar{A}(p) = \begin{pmatrix} \bar{A}_{pp} & 0 \\ 0 & \bar{A}_{\bar{p}\bar{p}} \end{pmatrix}$$

Simplify the connection (valid if $\langle\Phi_0\,|\,\Phi_1\rangle = 0$)

$$\tilde{\beta}_\nu^+ = \bar{A}_{\nu\nu}\, \tilde{\alpha}_\nu^+ + \bar{B}_{\bar{\nu}\nu}\, \tilde{\alpha}_{\bar{\nu}}$$

$$|\Phi_1\rangle = \tilde{\mathcal{C}}_{01} \prod (\bar{A}_{pp}^* + \bar{B}_{p\bar{p}}^*\, \tilde{\alpha}_p^+ \tilde{\alpha}_{\bar{p}}^+)\,|\Phi_0\rangle$$

Ring and Schuck Book

Some Theorem made simple

$$|\Phi_1\rangle = \tilde{\mathcal{C}}_{01} \prod \left(\bar{A}^*_{pp} + \bar{B}^*_{p\bar{p}}\, \tilde{\alpha}^+_p \tilde{\alpha}^+_{\bar{p}}\right) |\Phi_0\rangle$$

Overlaps ➡

$$\langle\Phi_0|\Phi_1\rangle = \tilde{\mathcal{C}}_{01} \prod \bar{A}^*_{pp} = \tilde{\mathcal{C}}_{01}\sqrt{\det(\bar{A}^*)}$$

(Onishi-Yoshida)

Thouless Theorem ➡

if $\bar{A}^*_{pp} \neq 0$ ***We define*** $\bar{Z}_{p\bar{p}} = (\bar{B}_{p\bar{p}}\bar{A}^{-1}_{pp})^*$

$$\begin{aligned} \rightarrow |\Phi_1\rangle &= \tilde{\mathcal{C}}_{01} \prod \bar{A}^*_{pp} \left(1 + \bar{Z}_{p\bar{p}}\, \tilde{\alpha}^+_p \tilde{\alpha}^+_{\bar{p}}\right) |\Phi_0\rangle \\ &= \mathcal{N}_{01}\, e^{\sum_p \bar{Z}_{p\bar{p}}\, \tilde{\alpha}^+_p \tilde{\alpha}^+_{\bar{p}}} |\Phi_0\rangle \end{aligned}$$

Expectation values ➡

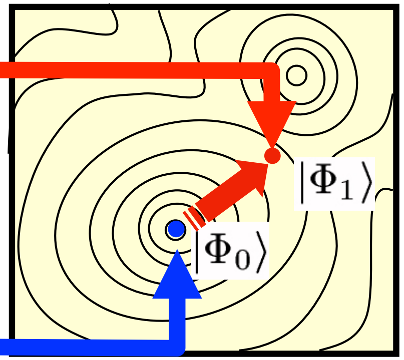
$$\begin{aligned} \langle\Phi_0|\tilde{\alpha}^+_\nu \tilde{\alpha}_\mu|\Phi_1\rangle &= \langle\Phi_0|\tilde{\alpha}^+_\nu \tilde{\alpha}^+_\mu|\Phi_1\rangle = 0 \\ \langle\Phi_0|\tilde{\alpha}_\nu \tilde{\alpha}^+_\mu|\Phi_1\rangle &= \delta_{\nu\mu}\langle\Phi_0|\Phi_1\rangle\ , \\ \langle\Phi_0|\tilde{\alpha}_\nu \tilde{\alpha}_\mu|\Phi_1\rangle &= \delta_{\bar{\nu}\mu}\, \bar{B}^*_{\bar{\nu}\nu}\langle\Phi_0|\Phi_1,\nu\rangle \end{aligned}$$

with $\langle\Phi_0|\Phi_1, p\rangle \equiv \tilde{\mathcal{C}}_{01} \prod_{p'\neq p} \bar{A}^*_{p'p'}$

$$\begin{aligned} \rho^{01} &= \rho^{00} + \tilde{U}^0\, \bar{Z}\, \tilde{V}^{0\,T} \\ \kappa^{01} &= \kappa^{00} + \tilde{U}^0\, \bar{Z}\, \tilde{U}^{0\,T} \\ \kappa^{10^*} &= \kappa^{00^*} - \tilde{V}^0\, \bar{Z}\, \tilde{V}^{0\,T} \end{aligned}$$

MR

SR



Recovering the Generalized Wick Theorem

and sources of difficulties in the GWT+EDF

Notations $\langle\Phi_0|\Phi_1\rangle = \bar{A}_{\nu\nu}\langle\Phi_0|\Phi_1,\nu\rangle = \bar{A}_{\nu\nu}\bar{A}_{\mu\mu}\langle\Phi_0|\Phi_1,\nu,\mu\rangle$

with $\langle\Phi_0|\Phi_1,\nu\rangle = \langle\Phi_0|\Phi_1,\bar{\nu}\rangle$ *and* $\langle\Phi_0|\Phi_1,\nu,\nu\rangle = \langle\Phi_0|\Phi_1,\nu,\bar{\nu}\rangle = 0$

$$\langle\Phi_0|\hat{V}_{12}|\Phi_1\rangle_{Direct}$$

Summary of pathologies

SR

$$+\frac{1}{2}\sum_{\nu\mu ijkl}\tilde{V}^{0}_{i\nu}\tilde{V}^{0}_{j\mu}\tilde{V}^{0*}_{l\mu}\tilde{V}^{0*}_{k\nu}\,\bar{v}^{\rho\rho}_{ijkl}\langle\Phi_0|\Phi_1\rangle$$

← **SR- self-interaction**

MR

$$+\frac{1}{2}\sum_{\nu\mu ijkl}\tilde{V}^{0}_{i\nu}\tilde{V}^{0}_{j\mu}\tilde{V}^{0*}_{l\mu}\tilde{U}^{0}_{k\bar{\nu}}\,\bar{v}^{\rho\rho}_{ijkl}\bar{B}^{*}_{\bar{\nu}\nu}\langle\Phi_0|\Phi_1,\nu\rangle$$

$$+\frac{1}{2}\sum_{\nu\mu ijkl}\tilde{V}^{0}_{i\nu}\tilde{V}^{0}_{j\mu}\tilde{U}^{0}_{l\bar{\mu}}\tilde{V}^{0*}_{k\nu}\,\bar{v}^{\rho\rho}_{ijkl}\bar{B}^{*}_{\bar{\mu}\mu}\langle\Phi_0|\Phi_1,\mu\rangle$$

$$+\frac{1}{2}\sum_{\nu\mu ijkl}\tilde{V}^{0}_{i\nu}\tilde{V}^{0}_{j\mu}\tilde{U}^{0}_{l\bar{\mu}}\tilde{U}^{0}_{k\bar{\nu}}\,\bar{v}^{\rho\rho}_{ijkl}\bar{B}^{*}_{\bar{\nu}\nu}\bar{B}^{*}_{\bar{\mu}\mu}\langle\Phi_0|\Phi_1,\nu,\mu\rangle$$

← } **MR self-inter /self-pairing** ← **Diverg.**

SR

$$+\frac{1}{4}\sum_{\nu\mu ijkl}\tilde{V}^{0}_{i\nu}\tilde{U}^{0*}_{j\nu}\tilde{U}^{0}_{l\mu}\tilde{V}^{0*}_{k\mu}\,\bar{v}^{\kappa\kappa}_{ijkl}\langle\Phi_0|\Phi_1\rangle$$

← **SR-self-inter /self-pairing**

MR

$$+\frac{1}{4}\sum_{\nu\mu ijkl}\tilde{V}^{0}_{i\nu}\tilde{V}^{0}_{j\bar{\nu}}\tilde{U}^{0}_{l\mu}\tilde{V}^{0*}_{k\mu}\,\bar{v}^{\kappa\kappa}_{ijkl}\bar{B}^{*}_{\bar{\nu}\nu}\langle\Phi_0|\Phi_1,\nu\rangle$$

$$+\frac{1}{4}\sum_{\nu\mu ijkl}\tilde{V}^{0}_{i\nu}\tilde{U}^{0}_{j\nu}\tilde{U}^{0}_{l\mu}\tilde{U}^{0}_{k\bar{\mu}}\,\bar{v}^{\kappa\kappa}_{ijkl}\bar{B}^{*}_{\bar{\mu}\mu}\langle\Phi_0|\Phi_1,\mu\rangle$$

$$+\frac{1}{4}\sum_{\nu\mu ijkl}\tilde{V}^{0}_{i\nu}\tilde{V}^{0}_{j\bar{\nu}}\tilde{U}^{0}_{l\mu}\tilde{U}^{0}_{k\bar{\mu}}\,\bar{v}^{\kappa\kappa}_{ijkl}\bar{B}^{*}_{\bar{\nu}\nu}\bar{B}^{*}_{\bar{\mu}\mu}\langle\Phi_0|\Phi_1,\nu,\mu\rangle$$

← } **MR self-inter /self-pairing** ← **Diverg.**

Practical and conceptual difficulties in Configuration Mixing within EDF

(I) Lacroix, et al, PRC79 (2009), (II) Bender et al PRC79 (2009), (III) Duguet et al, PRC79 (2009).

Correction is possible

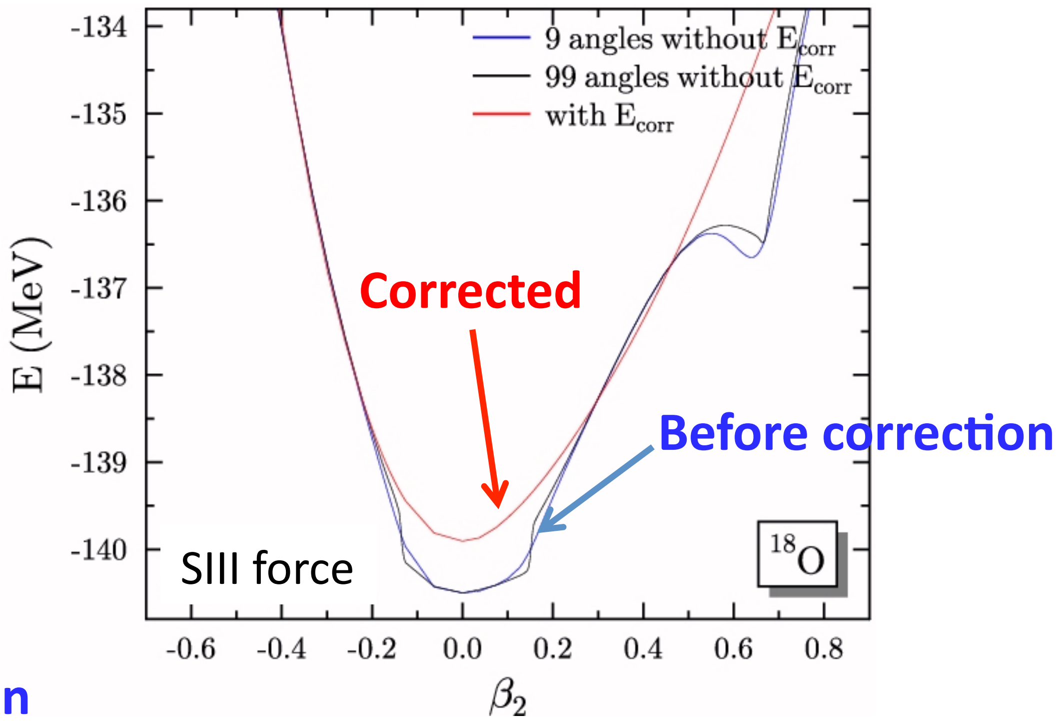
$$\mathcal{E} = \mathcal{E}^{\rho} + \mathcal{E}^{\rho\rho} + \mathcal{E}^{\kappa\kappa} + \cdots$$

with

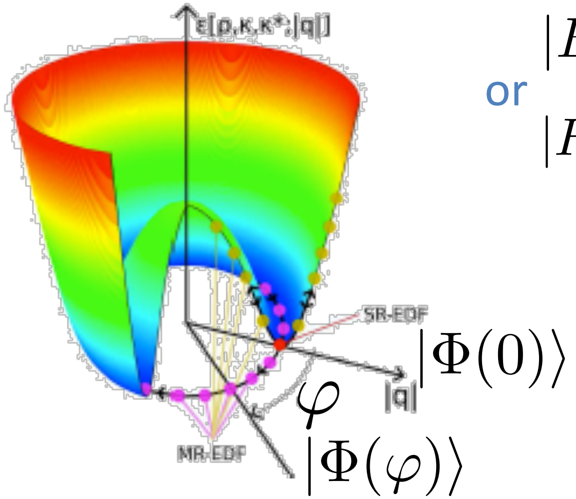
$$\mathcal{E}^{\rho\rho} \rightarrow \mathcal{E}^{\rho\rho} - \mathcal{E}^{\rho\rho}{}_{\mathrm{Corr.}}$$

$$\mathcal{E}^{\kappa\kappa} \rightarrow \mathcal{E}^{\kappa\kappa} - \mathcal{E}^{\kappa\kappa}{}_{\mathrm{Corr.}}$$

. . . .



Example: particle number projection



$$|BCS\rangle \text{ or } |HFB\rangle = \prod_{p>0} (u_p + v_p a_p^{\dagger} a_{\bar{p}}^{\dagger})|-\rangle$$

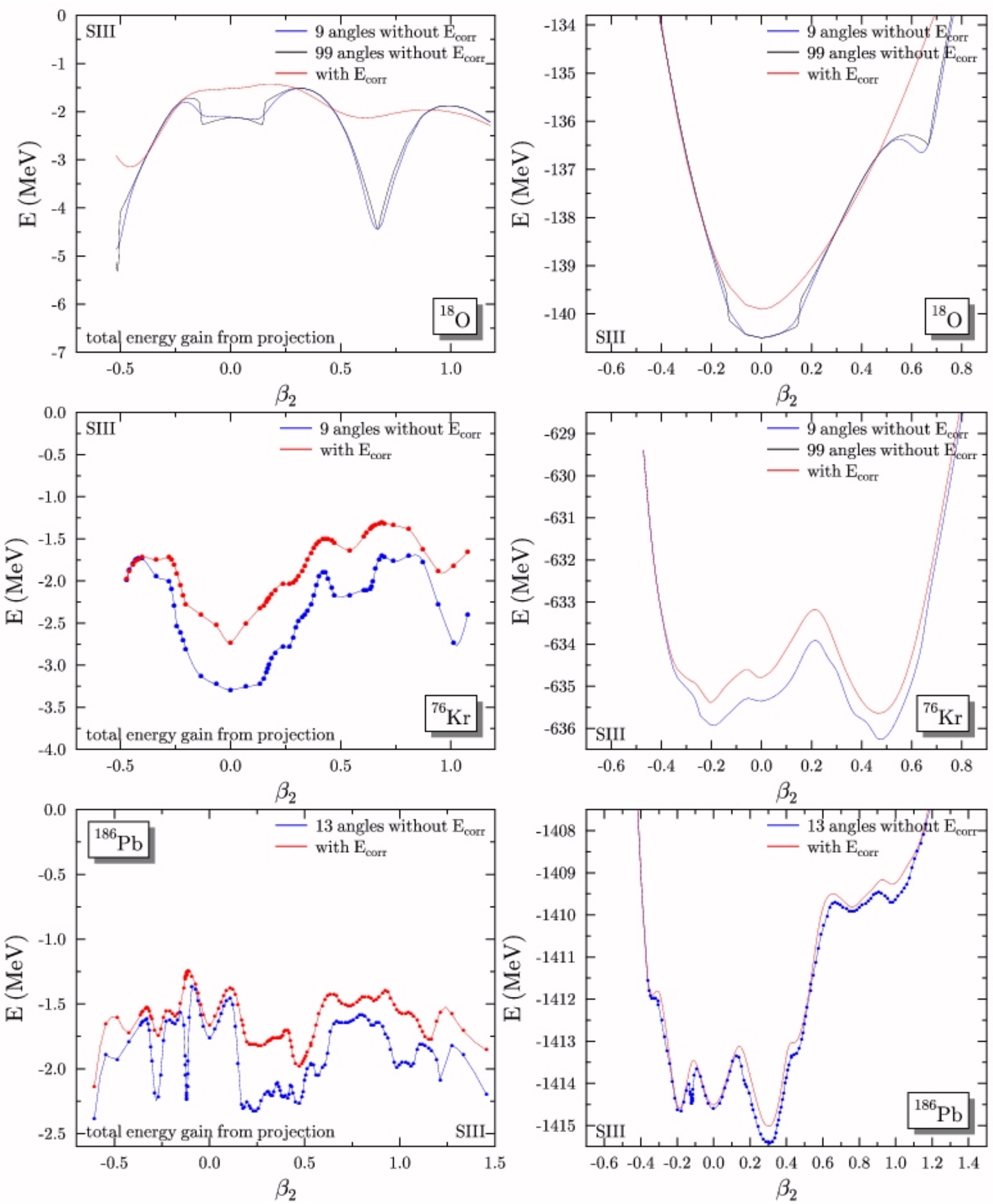
Lacroix et al, PRC79 (2009)
Bender et al, PRC79 (2009)
Duguet et al, PRC79 (2009)

Projection on
Good particle number

$$|N\rangle = \int_0^{2\pi} d\varphi \, \frac{e^{-i\varphi N}}{2\pi \, c_N} |\Phi[\varphi]\rangle$$

with $|\Phi[\varphi]\rangle = e^{i\varphi \hat{N}} |\Phi_0\rangle$

More results of the correction



➡ **Correction strongly Constraint the functional**

only ρ, ρ², ρ³, ρ⁴, ρ⁵ could be used

No ρ^α !!!

➡ **Correction leads to a new functional**

➡ **Application to other Symmetry breaking**

See M. Bender talk

Summary on correction of problem in EDF:

General EDF framework

Keep the full Power of EDF
-Phenomenological terms
-Different pp and ph interactions
-Exchange

-Self-interaction in SR and MR
-Divergences in conf. mixing

-Corrections are possible with different pp and ph interactions
-Limit the type of terms

Effective Hamiltonian

-Same pp and ph interaction.
-Exchange and coulomb fully treated
➡ Closer to an Hamiltonian approach

Anguiano et al, NPA 696 (2001)

-No Divergences
-But EDF is ill defined: (shift invariance)

Requires a constructive framework for EDF:

1-to construct Single-Ref EDF
2-To extend to conf. mixing
3-Require major changes in codes

4-MR-EDF as a functional theory?

Configuration mixing as a functional theory

The two-body Hamiltonian case: what is a functional of what?

$$H = \sum_{ij} t_{ij}\, a_i^\dagger\, a_j + \frac{1}{4}\sum_{ijkl} \bar{v}_{ijkl}\, a_i^\dagger\, a_j^\dagger\, a_l\, a_k$$

Mean-Field (with Pairing)

$$|\Phi_0\rangle = \Pi \beta_\alpha^\dagger |-\rangle$$

$$\langle H \rangle = \sum_i t_{ii}\rho_{ii} + \frac{1}{2}\sum_{i,j} \bar{v}_{ijij}\rho_{ii}\rho_{jj} + \frac{1}{4}\sum_{i,j} \bar{v}_{i\bar{i}j\bar{j}}\kappa_{i\bar{i}}^*\kappa_{j\bar{j}}$$
$$= E_{SR}[\rho, \kappa, \kappa^*]$$

$$\Phi_0 \to \{\rho, \kappa\} \to E_{SR}$$

Projection

$$|\Psi_\Omega\rangle = P^\Omega |\Phi_0\rangle$$
$$= \int dQ f(Q) |\Phi(Q)\rangle$$

$$E_{MR} = \iint dQ dQ' \mathcal{N}(Q,Q') E_{SR}(\rho^{QQ'}, \kappa^{QQ'}, \kappa^{*QQ'})$$

Alternative formulation

$$|\Psi_\Omega\rangle = P^\Omega |\Phi_0\rangle$$

$$E_{MR} = \sum t_{ij}\, \langle a_i^\dagger\, a_j \rangle_\Omega + \frac{1}{4}\sum \bar{v}_{ijkl}\langle a_i^\dagger\, a_j^\dagger\, a_l\, a_k\rangle_\Omega$$

$$E_{MR} = \sum_{ij} t_{ij}\, \rho_{ij}^\Omega + \frac{1}{4}\sum_{ijkl} \bar{v}_{ijkl} R_{kl,ij}^\Omega$$

$$\Phi_0 \to \{\rho^{QQ'}, \kappa^{QQ'}, \kappa^{*QQ'}\} \to E_{MR} \quad \Longleftrightarrow \quad \Phi_0 \to \Psi_\Omega \to \{\rho^\Omega, R^\Omega\} \to E_{MR}$$

What about the EDF theory?

The particle number restoration case

$$|\Psi_N\rangle = P^N|\Phi_0\rangle$$

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

Mean-Field (with Pairing)

$$|\Phi_0\rangle = \Pi\beta^\dagger_\alpha|-\rangle$$

$$\mathcal{E}_{SR}\left[\rho,\kappa,\kappa^*\right] = \sum t_{ii}\rho_{ii} + \frac{1}{2}\sum \overline{v}^{\rho\rho}_{ijij}\rho_{ii}\rho_{jj} + \frac{1}{4}\sum \overline{v}^{\kappa\kappa}_{i\bar{i}j\bar{j}}\kappa^*_{i\bar{i}}\kappa_{j\bar{j}}$$

$$\Phi_0 \rightarrow \{\rho,\kappa\} \rightarrow \mathcal{E}_{SR}$$

Projection

$$\mathcal{E}_N[\Psi_N] \equiv \int_0^{2\pi} d\varphi\, \mathcal{E}_{SR}\left[\rho^{0\varphi},\kappa^{0\varphi},\kappa^{\varphi 0^\star}\right]\mathcal{N}_N(0,\varphi)$$

$$\Phi_0 \rightarrow \{\rho^{0\varphi},\kappa^{0\varphi},\kappa^{*0\varphi}\} \rightarrow \mathcal{E}_N$$

Alternative formulation ?

For non-density dependent effective int.

$$\mathcal{E}_N[\Psi_N] = \sum_i t_{ii}n^N_i + \frac{1}{2}\sum_{i,j,j\neq\bar{i}} \overline{v}^{\rho\rho}_{ijij}R^N_{ijij} + \frac{1}{4}\sum_{i\neq j,i\neq\bar{j}} \overline{v}^{\kappa\kappa}_{i\bar{i}j\bar{j}}R^N_{j\bar{j}i\bar{i}}$$

OK

$$+ \frac{1}{2}\sum_i \overline{v}^{\rho\rho}_{i\bar{i}i\bar{i}}\int_0^{2\pi} d\varphi\; n^{0\varphi}_i\; n^{0\varphi}_i\mathcal{N}_N(0,\varphi) + \frac{1}{2}\sum_i \overline{v}^{\kappa\kappa}_{i\bar{i}i\bar{i}}\int_0^{2\pi} d\varphi\kappa^{\varphi 0^\star}_{i\bar{i}}\;\kappa^{0\varphi}_{i\bar{i}}\;\mathcal{N}_N(0,\varphi),$$

?

Terms that needs to be corrected

The particle number restoration case

$$|\Psi_N\rangle = P^N |\Phi_0\rangle$$

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

Mean-Field (with Pairing)

$$|\Phi_0\rangle = \Pi \beta^\dagger_\alpha |-\rangle$$

$$\mathcal{E}_{SR}[\rho,\kappa,\kappa^*] = \sum t_{ii}\rho_{ii} + \frac{1}{2}\sum \overline{v}^{\rho\rho}_{ijij}\rho_{ii}\rho_{jj} + \frac{1}{4}\sum \overline{v}^{\kappa\kappa}_{i\bar{i}j\bar{j}}\kappa^*_{i\bar{i}}\kappa_{j\bar{j}}$$

$$\Phi_0 \rightarrow \{\rho,\kappa\} \rightarrow \mathcal{E}_{SR}$$

Projection

$$\mathcal{E}_N[\Psi_N] \equiv \int_0^{2\pi} d\varphi \, \mathcal{E}_{SR}\left[\rho^{0\varphi},\kappa^{0\varphi},\kappa^{\varphi 0\star}\right]\mathcal{N}_N(0,\varphi)$$

$$\Phi_0 \rightarrow \{\rho^{0\varphi},\kappa^{0\varphi},\kappa^{*0\varphi}\} \rightarrow \mathcal{E}_N$$

Alternative formulation ?

For non-density dependent effective int.

After regularization proposed in

Lacroix, Duguet, Bender, PRC79 (2009)

$$\mathcal{E}_N[\Psi_N] = \sum_i t_{ii} n_i^N + \frac{1}{2}\sum_{i,j,j\neq\bar{i}} \overline{v}^{\rho\rho}_{ijij} R^N_{ijij} + \frac{1}{4}\sum_{i\neq j,j\neq\bar{i}} \overline{v}^{\kappa\kappa}_{i\bar{i}j\bar{j}} R^N_{j\bar{j}i\bar{i}} + \frac{1}{2}\sum_i \overline{v}^{\rho\rho}_{i\bar{i}i\bar{i}}(n_i^N n_i^N - \delta n_i \delta n_i) + \frac{1}{2}\sum_i \overline{v}^{\kappa\kappa}_{i\bar{i}i\bar{i}}\left[n_i^N(1-n_i^N) + \delta n_i \delta n_i\right],$$

OK

$$\delta n_i = n_i^N - n_i^0$$

Ψ_N $\qquad$ Φ_0

The particle number restoration case

$$|\Psi_N\rangle = P^N|\Phi_0\rangle$$

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

Mean-Field (with Pair

Alternative formulation ?

sity dependent effective int.

rization proposed in

Lacroix, Duguet, Bender, PRC7 (2009)

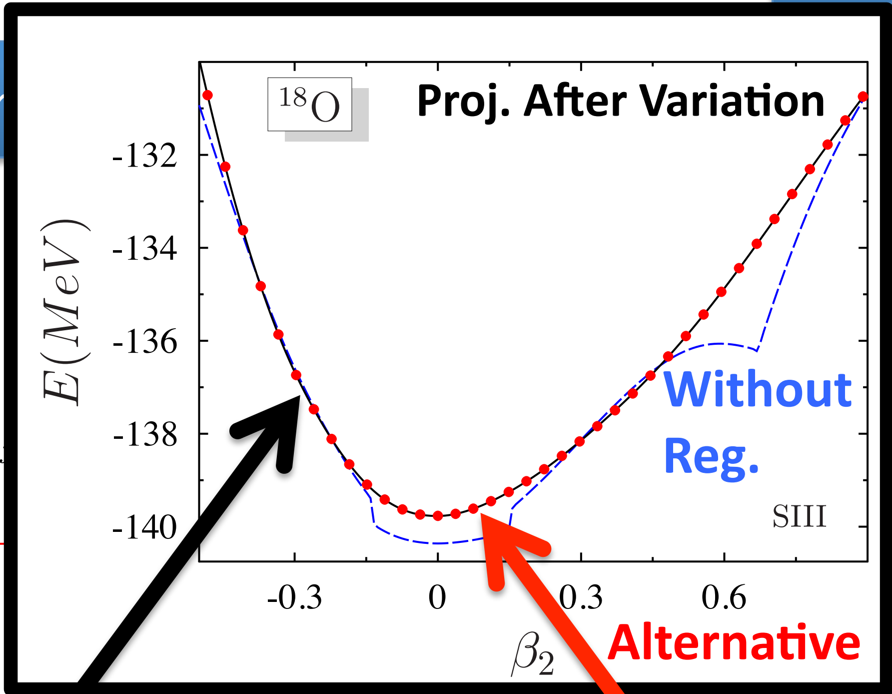
$$|\Phi_0\rangle = \Pi \beta_\alpha^\dagger |-\rangle$$

$$\mathcal{E}_{SR}[\rho,\kappa,\kappa^*] = \sum t_{ii}\rho_{ii}$$

$$+\frac{1}{2}\sum \overline{v}^{\rho\rho}_{ijij}$$

$\Phi_0 \to \{\rho, \kappa\}$ –

Projection



$$t_{ii} n_i^N$$

$$\sum_{,j,j\neq\bar{i}} \overline{v}^{\rho\rho}_{ijij} R^N_{ijij}$$

$$\sum_{\neq j,j\neq\bar{i}} \overline{v}^{\kappa\kappa}_{i\bar{i}j\bar{j}} R^N_{j\bar{j}i\bar{i}}$$

$$+\frac{1}{2}\sum_i \overline{v}^{\rho\rho}_{i\bar{i}i\bar{i}}(n_i^N n_i^N - \delta n_i \delta n_i)$$

$$+\frac{1}{2}\sum_i \overline{v}^{\kappa\kappa}_{i\bar{i}i\bar{i}}\left[n_i^N(1-n_i^N) + \delta n_i \delta n_i\right],$$

OK

$$\mathcal{E}_N[\Psi_N] \equiv \int_0^{2\pi} d\varphi\, \mathcal{E}_{SR}\left[\rho^{0\varphi}, \kappa^{0\varphi}, \kappa^{\varphi 0 \star}\right] \mathcal{N}_N(0,\varphi)$$

$$\delta n_i = n_i^N - n_i^0$$

Ψ_N Φ_0

$$\Phi_0 \to \{\rho^{0\varphi}, \kappa^{0\varphi}, \kappa^{*0\varphi}\} \to \mathcal{E}_N$$

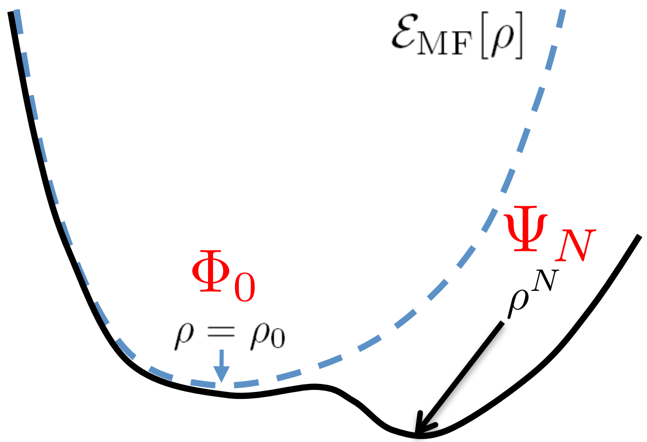
Hupin, Lacroix, Bender, PRC(2011)

Direct formulation:

$$\Psi_N \rightarrow \{\rho^N, R^N\} \rightarrow \mathcal{E}_{SC}(\rho^N, R^N)$$

Advantages

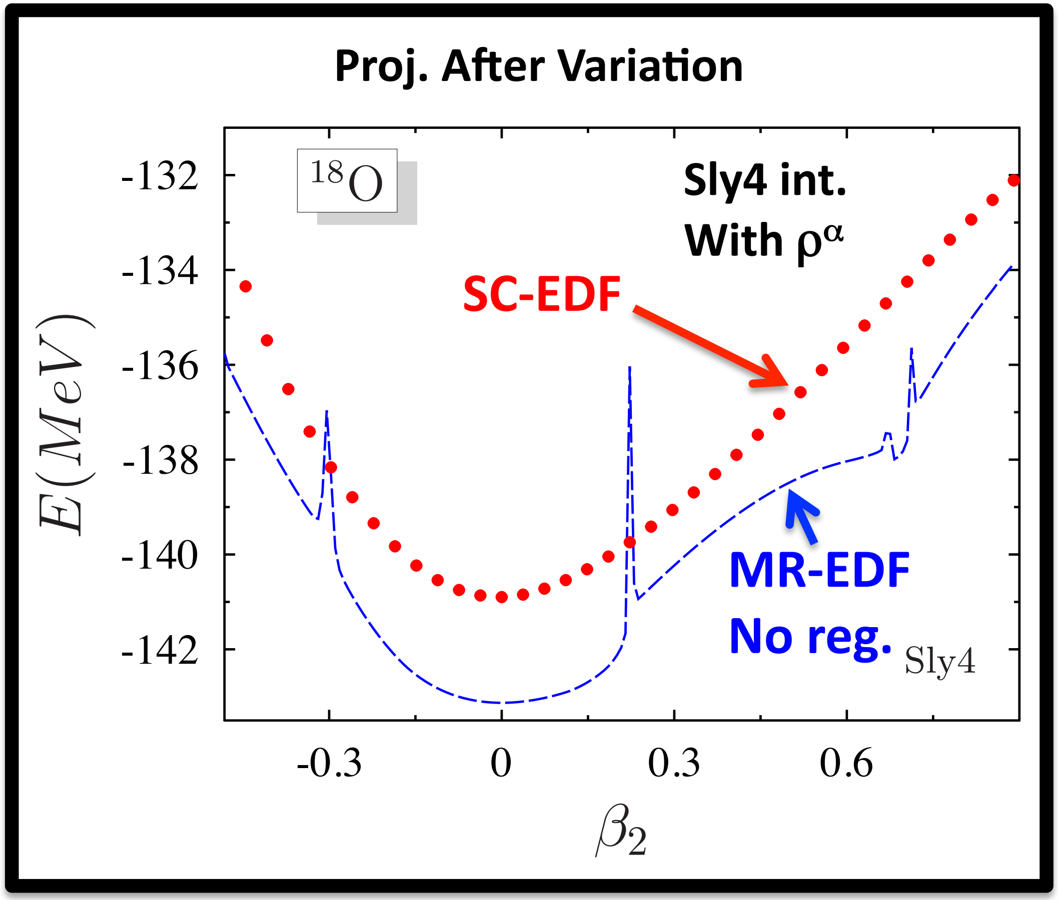
- the functional is automatically symmetry conserving.
- It is equivalent to MR-EDF for non density dependent term
- It is a natural extension of SR-EDF



- It is free of jumps/divergence

(Full VAP minimization possible : G. Hupin talk)

Hupin, Lacroix, Bender, PRC(2011) arXiv 1105.4084



- It could be extended to dens. dependent interaction

$$\overline{v}^{\rho\rho}[\rho] \Longrightarrow \overline{v}^{\rho\rho}[\rho^N], \quad \overline{v}^{\kappa\kappa}[\rho] \Longrightarrow \overline{v}^{\kappa\kappa}[\rho^N]$$

Strategies to restore symmetries within EDF

Multi-Reference strategy

$$\Phi_0 \rightarrow \{\rho^{0\varphi}, \kappa^{0\varphi}, \kappa^{*0\varphi}\} \rightarrow \mathcal{E}_N$$

- Projection and excited states
- Requires off-diagonal energy kernels
- Requires tedious regularization
  Does not seems trivial to apply
  For any symmetry breaking
- Very restrictive for the functional to be used

Single-Reference strategy

$$\Psi_N \rightarrow \{\rho^N, R^N\} \rightarrow \mathcal{E}_{SC}(\rho^N, R^N)$$

- For lowest state only
- No off-diagonal energy kernels
- Large flexibility for the functional choice
- Application to other symmetries ?

$$\Psi = \int dQ f(Q) |\Phi(Q)\rangle \rightarrow \{\rho^1, R^2\} \rightarrow \mathcal{E}_{Mix}$$

Stick on the Hamiltonian case?