t1

Nuclear Energy Density Functional Method

How to (safely…) account for correlations in ground and excited states of heavy nuclei?

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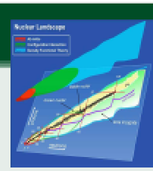
Slide 1

t1 tduguet, 5/21/2008

Ultimate goals

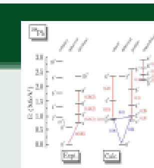
Ground state

Mass, deformation



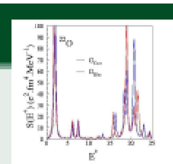
Spectroscopy

Spectroscopy



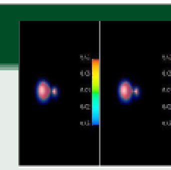
Collective modes

RPA, QRPA, GCM



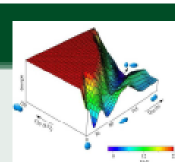
Reaction properties

Fusion, transfer, elastic



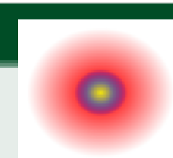
Heavy elements

Fission, fusion, SHE



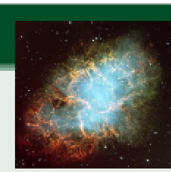
Exotic behaviors

Drip-lines, halos



Astrophysics

r-process, NS, SN



From underlying NN and NNN interactions

Nuclear EDF method: key points

I EDF method addresses both ground and excited states

One single energy functional

Two levels of many-body implementations

- Single reference
- Multi reference

II EDF method addresses both structure and reactions properties

Two different schemes

- Time independent for stucture properties
- Time dependent for structure and reaction properties

III EDF method is currently transitioning from empirical to non/less empirical

Energy kernel(s) so far built by analogy with matrix elements of fictitious « H »

- Base-line and insights from strict « H »-based approach
- EDF extends it empirically to grasp additional necessary correlations

Accuracy/predictive power of current empirical EDFs not sufficient/satisfactory

- Need to improve current phenomenology (e.g. M. Stoitsov, M. Kortelainen)
- Constrain EDF kernels from vacuum H and MBPT (e.g. T. Lesinski, B. Gebremariam)

Departure from « H »-based picture is at the origin of potentially serious problems

- **Need to better formulate the empirical method**
- Work needed to formulate the two-level EDF method from first principles

Single-Reference = « ~~Mean-field~~ »

I Formalism in a nutshell

$\mathcal{E}[\rho, \kappa, \kappa^*]$ = functional of one-body density matrices

$$\rho_{ji} = \langle \Phi | c_i^\dagger c_j | \Phi \rangle \quad ; \quad \kappa_{ji} = \langle \Phi | c_i c_j | \Phi \rangle$$

$|\Phi\rangle$ = auxiliary, **symmetry-breaking** product state (N, Z, J², P², Π)

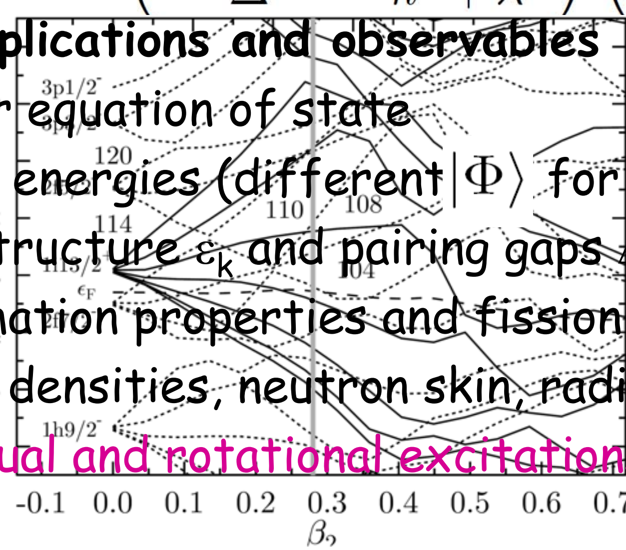
II Included correlations

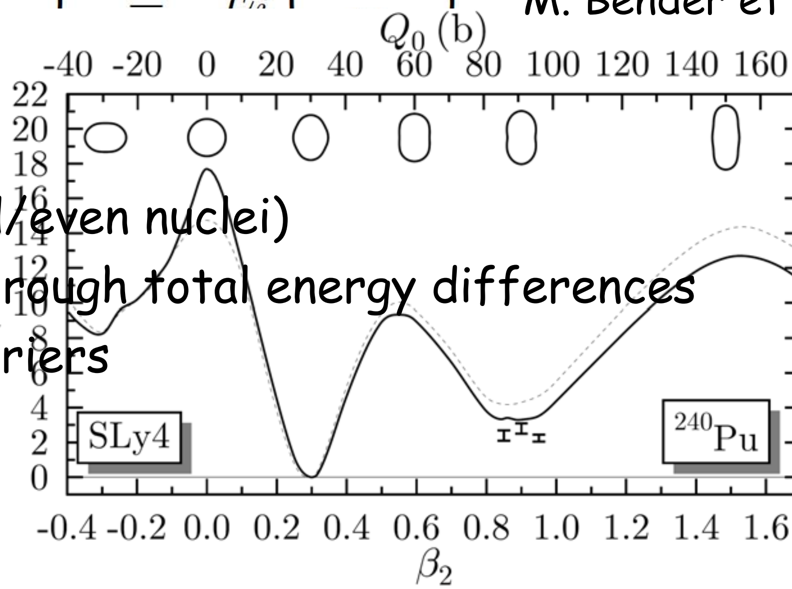
- « Bulk » ones into $\mathcal{E}[\rho, \kappa, \kappa^*]$ (~2nd order MBPT in infinite nuclear matter)
- « Static » collective ones through symmetry breaking (ρ and κ)
- Outside the frame of standard HK theorem of DFT

M. Bender et al.

III Applications and observables

- Nuclear equation of state
- Binding energies (different $|\Phi\rangle$ for odd/even nuclei)
- Shell structure ϵ_k and pairing gaps Δ_q through total energy differences
- Deformation properties and fission barriers
- Charge densities, neutron skin, radii
- Individual and rotational excitations





Standard energy functionals

I Functional form

- Skyrme is quasi-local / Gogny is non-local
- Skyrme's basic structure is bilinear in the following local densities

$\rho_q(\vec{r}) \equiv \sum_\sigma \rho_q(\vec{r}\sigma, \vec{r}\sigma)$	Matter density
$\tau_q(\vec{r}) \equiv \sum_\sigma \nabla \cdot \nabla' \rho_q(\vec{r}\sigma, \vec{r}\,'\sigma)\|_{\vec{r}=\vec{r}\,'}$	Kinetic density
$\vec{s}_q(\vec{r}) \equiv \sum_{\sigma\sigma'} \rho_q(\vec{r}\sigma, \vec{r}\,'\sigma)\, \vec{\sigma}_{\sigma'\sigma}$	Spin density
$\vec{j}_q(\vec{r}) \equiv \sum_\sigma i/2\ (\nabla' - \nabla)\ \rho_q(\vec{r}\sigma, \vec{r}\,'\sigma)\|_{\vec{r}=\vec{r}\,'}$	Current density
$\tilde{\rho}_q(\vec{r}) \equiv \sum_\sigma \kappa_q(\vec{r}\sigma, \vec{r}\bar{\sigma})\, \bar{\sigma}$	Pair density

II Basic features

- Symmetry rules to build allowed terms
- Simplistic density-dependent couplings at this point
- $\mathcal{E}[\rho,\kappa,\kappa^*] = \langle\Phi|"H"|\Phi\rangle/\langle\Phi|\Phi\rangle$ would tie Cs together/forbid dens.-dep. Cs
- **Universal** = applicable to *all nuclei* without local adjustment
- **Empirical** = no link to NN/NNN + fitted to experimental data

Multi-Reference = « Beyond ~~mean-field~~ »

I Formalism in a nutshell

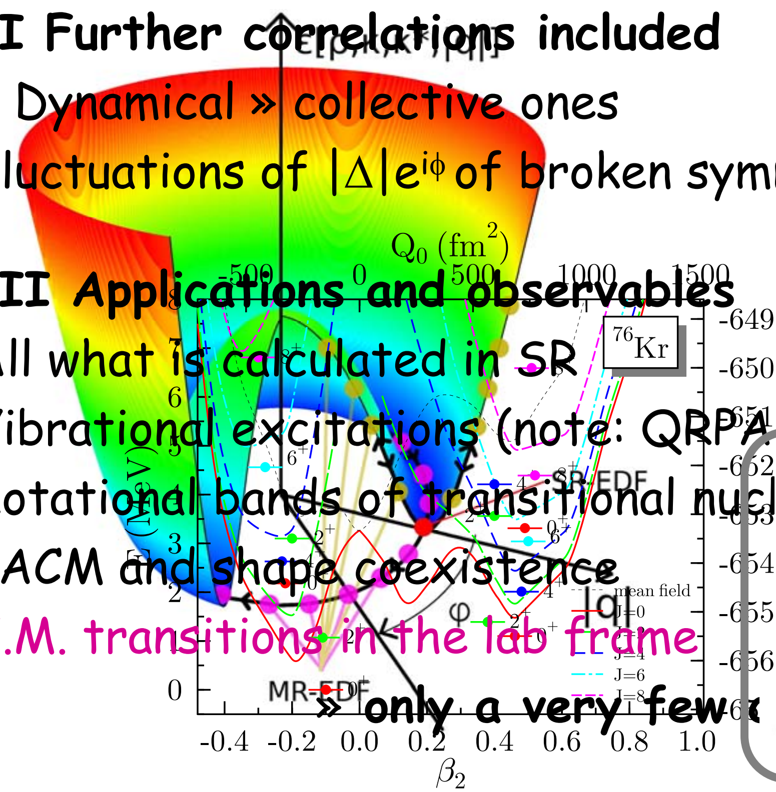
$\mathcal{E}[\rho^{01}, \kappa^{01}, \kappa^{10\,*}]$ = functional of one-body *transition* density matrices

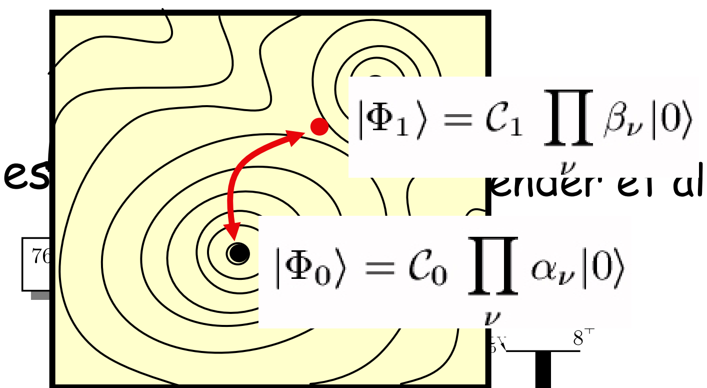
$$\rho^{01}_{ij} \equiv \frac{\langle \Phi_0 | a^+_j a_i | \Phi_1 \rangle}{\langle \Phi_0 | \Phi_1 \rangle} \qquad \kappa^{01}_{ij} \equiv \frac{\langle \Phi_0 | a_j a_i | \Phi_1 \rangle}{\langle \Phi_0 | \Phi_1 \rangle}$$

$\{|\Phi_0\rangle ; |\Phi_1\rangle\}$ = MR set of auxiliary, symmetry-breaking product states

II Further correlations included

- « Dynamical » collective ones
- Fluctuations of $|\Delta| e^{i\phi}$ of broken symmetries





III Applications and observables

- All what is calculated in SR
- Vibrational excitations (note: QRPA is a small amplitude limit of MR EDF)
- Rotational bands of transitional nucl
- LACM and shape coexistence
- E.M. transitions in the lab frame

» only a very few

$$\mathcal{E}^k \equiv \frac{\sum_{\{0,1\}\in \mathrm{MR}} f^{k\,*}_0 \, f^k_1 \, \mathcal{E}[0,1] \, \langle \Phi_0 | \Phi_1 \rangle}{\sum_{\{0,1\}\in \mathrm{MR}} f^{k\,*}_0 \, f^k_1 \, \langle \Phi_0 | \Phi_1 \rangle}$$

$$\mathcal{E}[0,1] \equiv \mathcal{E}[\rho^{01}, \kappa^{01}, \kappa^{10\,*}]$$

Some tricky points

I Should SR-EDF be final for gs and MR-EDF left for excited states?

Some practitioners believe so by analogy with DFT

- Symmetry breaking/restoring?
- Intrinsic DFT [J. Messud et al., arXiv:0904.0162]? For all symmetries? Is that convenient?

II Seems difficult in practice to account for dynamical correlations in SR-EDF

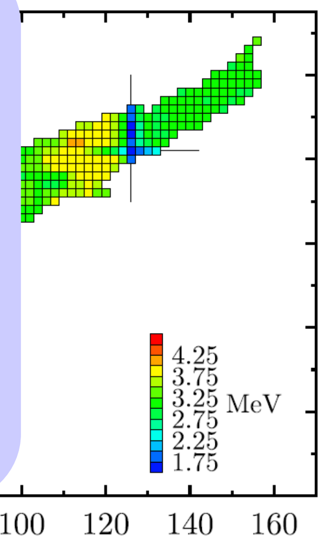
III Danger of double counting correlations

Splitting into « bulk/static/dynamical » not based on first principles

- There is no obvious separation of (energy) scales
- EDF built empirically and fitted at the SR level so far

Need to design a non-empirical framework

- On going effort as for building the SR-EDF from NN/NNN + MBPT
- But how does MR-EDF fits in? No first-principle backup so far



IV Unexpected, though very serious, additional difficulties…

Spurious divergencies and steps in PNR calculations

I Given the SR EDF

$$\mathcal{E}_{SR}[\rho^{00},\kappa^{00},\kappa^{00\,*}] = \sum_{ij} t_{ij}\,\rho^{00}_{ji} + \frac{1}{2}\sum_{ijkl}\bar{v}^{\rho\rho}_{ijkl}\,\rho^{00}_{ki}\,\rho^{00}_{lj} + \frac{1}{4}\sum_{ijkl}\bar{v}^{\kappa\kappa}_{ijkl}\,\kappa^{00\,*}_{ij}\,\kappa^{00}_{kl}$$

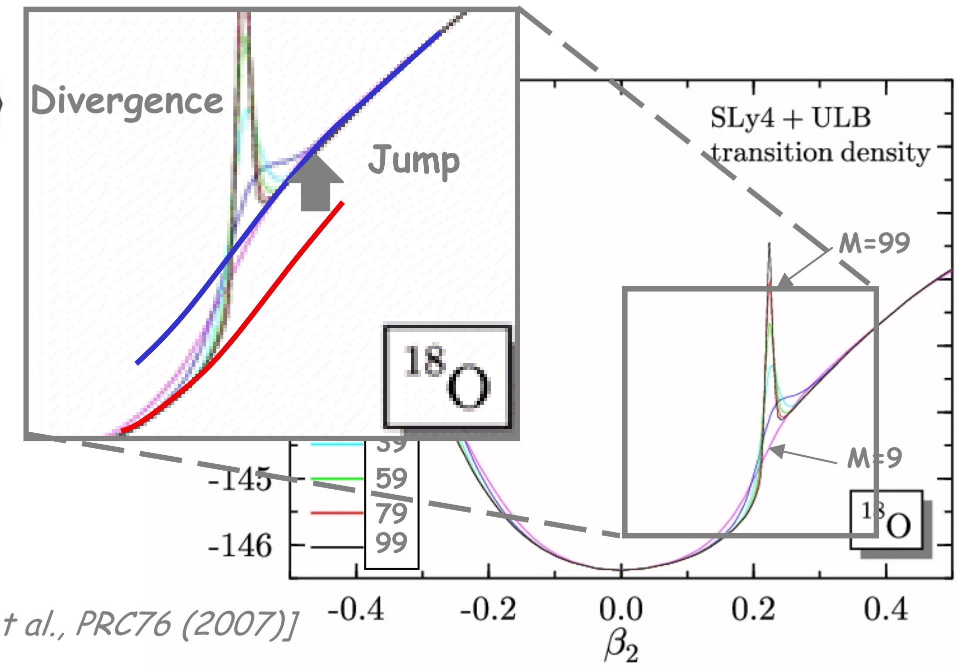
$$+\frac{1}{6}\sum_{ijklmn}\bar{v}^{\rho\rho\rho}_{ijklmn}\,\rho^{00}_{li}\,\rho^{00}_{mj}\,\rho^{00}_{nk} + \frac{1}{4}\sum_{ijklmn}\bar{v}^{\rho\kappa\kappa}_{ijklmn}\,\rho^{00}_{li}\,\kappa^{00\,*}_{jk}\,\kappa^{00}_{mn} + \ldots$$

II Particle Number Restoration: one particular MR mode

$$\mathcal{E}^{N} \equiv \int_0^{2\pi} d\varphi\,\frac{e^{-i\varphi N}}{2\pi\,c_N^2}\,\mathcal{E}_{MR}[\Phi_0,\Phi_\varphi]\,\langle\Phi_0|\Phi_\varphi\rangle$$

with the MR set

$$\begin{cases} |\Phi_\varphi\rangle \equiv e^{i\varphi\hat{N}}|\Phi_0\rangle \;;\; \varphi\in[0,2\pi] \\ \mathcal{E}_{MR}[\Phi_0,\Phi_\varphi] \equiv \mathcal{E}_{SR}[\rho^{0\varphi},\kappa^{0\varphi},\kappa^{\varphi 0\,*}] \end{cases}$$



[J. Dobaczewski et al., PRC76 (2007)]

But where does this prescription come from!?

[M. Bender, T. Duguet, IJMP E16 (2007)]

Definition of non-diagonal EDF kernels for MR calculations

the "nuclear physics strategy"

SR

MR

Hamiltonian based

Standard Wick Theorem (SWT)

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

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

Generalized Wick Theorem (GWT)

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

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

[B. Balian, E. Brezin, Nuovo Cimento 64 (1969))

EDF case

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

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

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

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

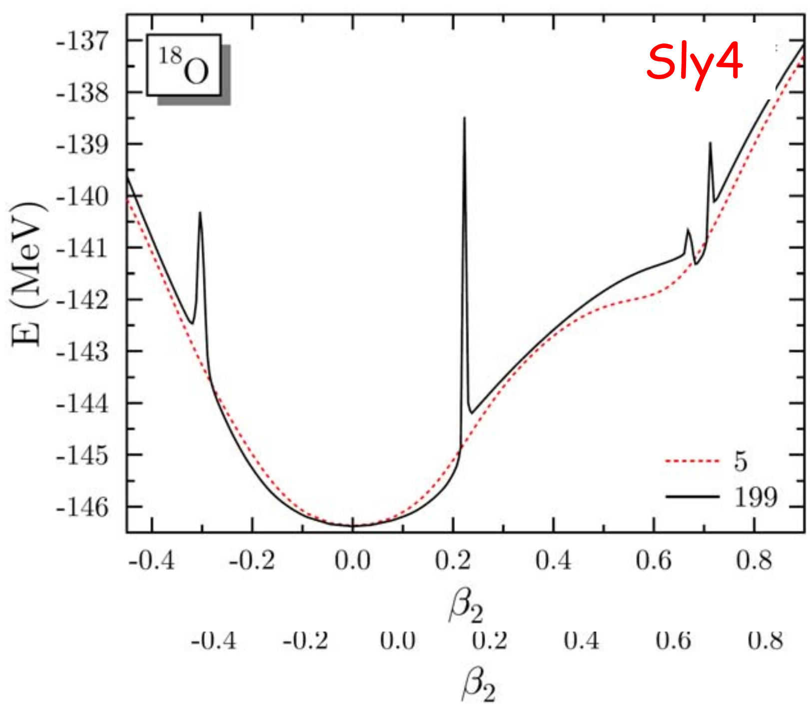
- ***Is the GWT-based extension procedure to be questioned in the EDF context?***
- ***If it is so, all MR modes and not only PNR should be compromised***
- ***Is there a safe and motivated alternative?***

The problem is indeed not specific to PNR

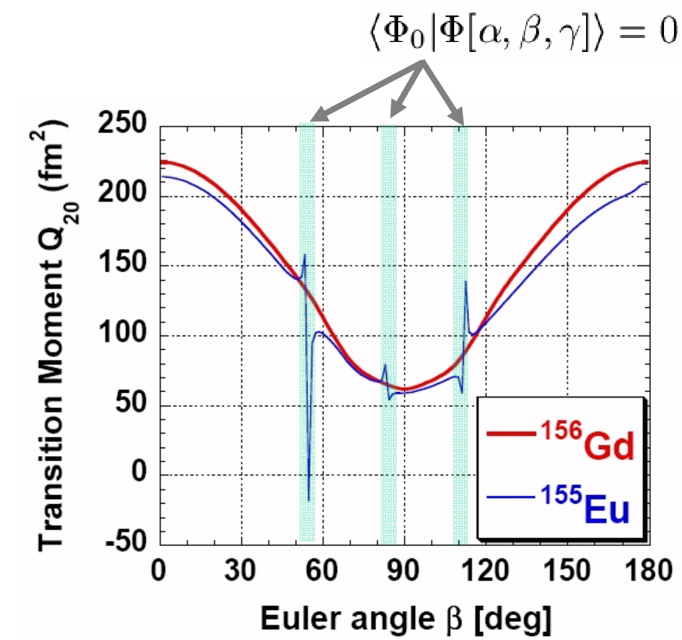
I Particle number restoration

EDF with non-integer power $\rho^{\gamma}\rho^{2}$

with integer powers



II Angular momentum restoration



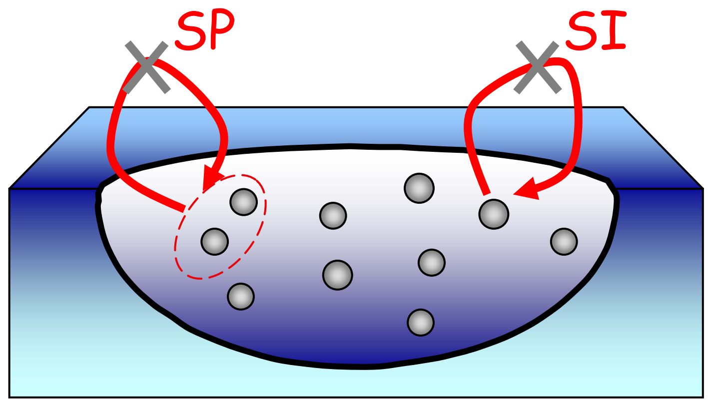
[H. Zdunczuk et al, IJMP E16 (2007)]

III Shape mixing

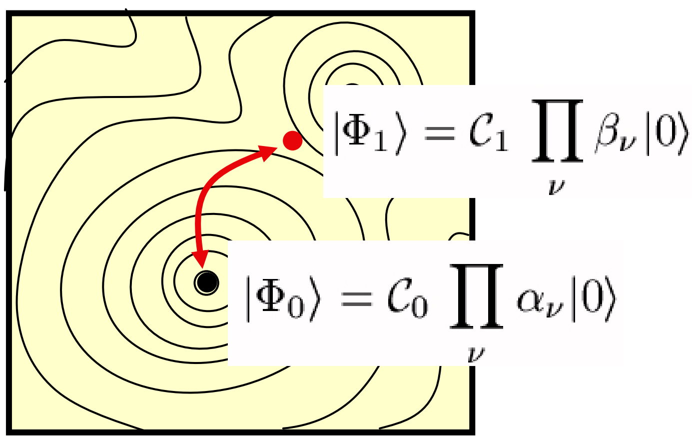
To be studied

(I) [D. Lacroix, T. Duguet, M. Bender,to appear in PRC; arXiv:0809.2041]

I Sources of pathologies



- Self-Interaction (SR+MR)
  - Not dramatic a priori
  - Need to be characterized
- Self-Pairing (SR+MR)
  - Not dramatic a priori
  - Need to be characterized
- GWT-motivated procedure within EDF framework (MR only)
  - Divergences, sharp steps, smooth steps plus kink



II Cure MR EDF kernels first

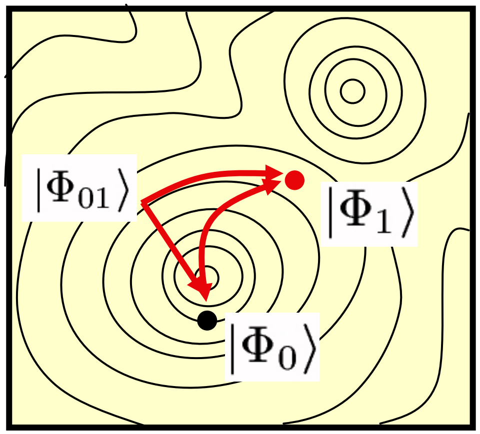
⇨ Find alternative to GWT

⇨ Identify critical terms

⇨ Remove pathologies in EDF case

Methods for connecting different quasi-particle vacua

(I) [D. Lacroix, T. Duguet, M. Bender, to appear in PRC; arXiv:0809.2041]



Starting point:

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

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

$$\alpha^+_\nu = \sum_i \left(U^0_{i\nu}\, a^+_i + V^0_{i\nu}\, a_i\right)$$

$$\beta^+_\nu = \sum_i \left(U^1_{i\nu}\, a^+_i + V^1_{i\nu}\, a_i\right)$$

$$\beta^+_\mu = \sum_\nu \left(A_{\nu\mu}\, \alpha^+_\nu + B_{\nu\mu}\, \alpha_\nu\right)$$

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

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

The Balian-Brezin (Thouless) strategy => GWT

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

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

The Bloch-Messiah-Zumino Strategy => SWT

Work directly on A and B

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

$$\alpha \xrightarrow{D} \tilde{\alpha} \qquad \beta \xrightarrow{C} \tilde{\beta}$$

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

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

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

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

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

Ring and Schuck Book

Interest of the Bloch-Messiah-Zumino technique

some Theorems made simple/recovered

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

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 →

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

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

Expectation values through SWT instead of GWT →

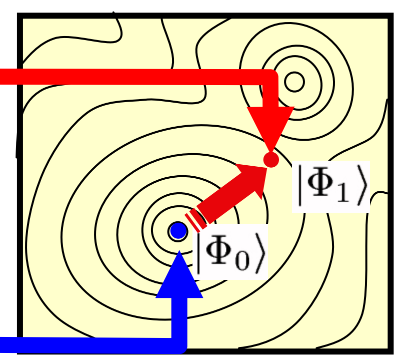
$$\begin{aligned}
\langle\Phi_0|\tilde{\alpha}^+_\nu \tilde{\alpha}_\mu|\Phi_1\rangle &= \langle\Phi_0|\tilde{\alpha}^+_\nu \tilde{\alpha}^+_\mu|\Phi_1\rangle = 0 \\
\langle\Phi_0|\tilde{\alpha}_\nu \tilde{\alpha}^+_\mu|\Phi_1\rangle &= \delta_{\nu\mu}\langle\Phi_0|\Phi_1\rangle \ , \\
\langle\Phi_0|\tilde{\alpha}_\nu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

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

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

MR

SR



Correct GWT-based definition of MR kernels

Strategy: compare SWT to GWT for MR kernel from "H" + extend to 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* $\langle \Phi_0 | \Phi_1, \nu, \nu \rangle = \langle \Phi_0 | \Phi_1, \nu, \bar{\nu} \rangle = 0$

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

SR

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

← SR- self-interaction

MR

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

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

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

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

SR

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

← SR-self-inter /self-pairing

MR

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

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

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

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

Summary of pathologies

- SR- self-interaction
- MR self-inter /self-pairing — Diverg/ step
- SR-self-inter /self-pairing
- MR self-inter /self-pairing — Diverg/ step

Practical regularization procedure

(I) [D. Lacroix, T. Duguet, M. Bender,to appear in PRC; arXiv:0809.2041]

I Start from a given SR EDF $\mathcal{E}_{SR}[\rho^{00}, \kappa^{00}, \kappa^{00\,*}]$
Can only depend on integer powers of the density *matrices*

II Consider a MR mode
Can be any combination modes allowed by the code

III Given $\{|\Phi_0\rangle; |\Phi_1\rangle\}$ **proceed to BMZ decomposition of Bogoliubov transfo**
To be done for each pair of reference states

IV Define $\mathcal{E}_{MR}[\Phi_0, \Phi_1] \equiv \mathcal{E}_{SR}[\rho^{01}, \kappa^{01}, \kappa^{10\,*}]$ **and subtract spurious terms**
Leaves SR EDF untouched

First application: particle number restoration

(II) [M. Bender, T. Duguet, D. Lacroix, to appear in PRC, arXiv:0809.2045]

I Step III above is trivial in this particular case

II Terms to be removed from $\mathcal{E}_{MR}[\Phi_0, \Phi_\varphi]$

ρρ term

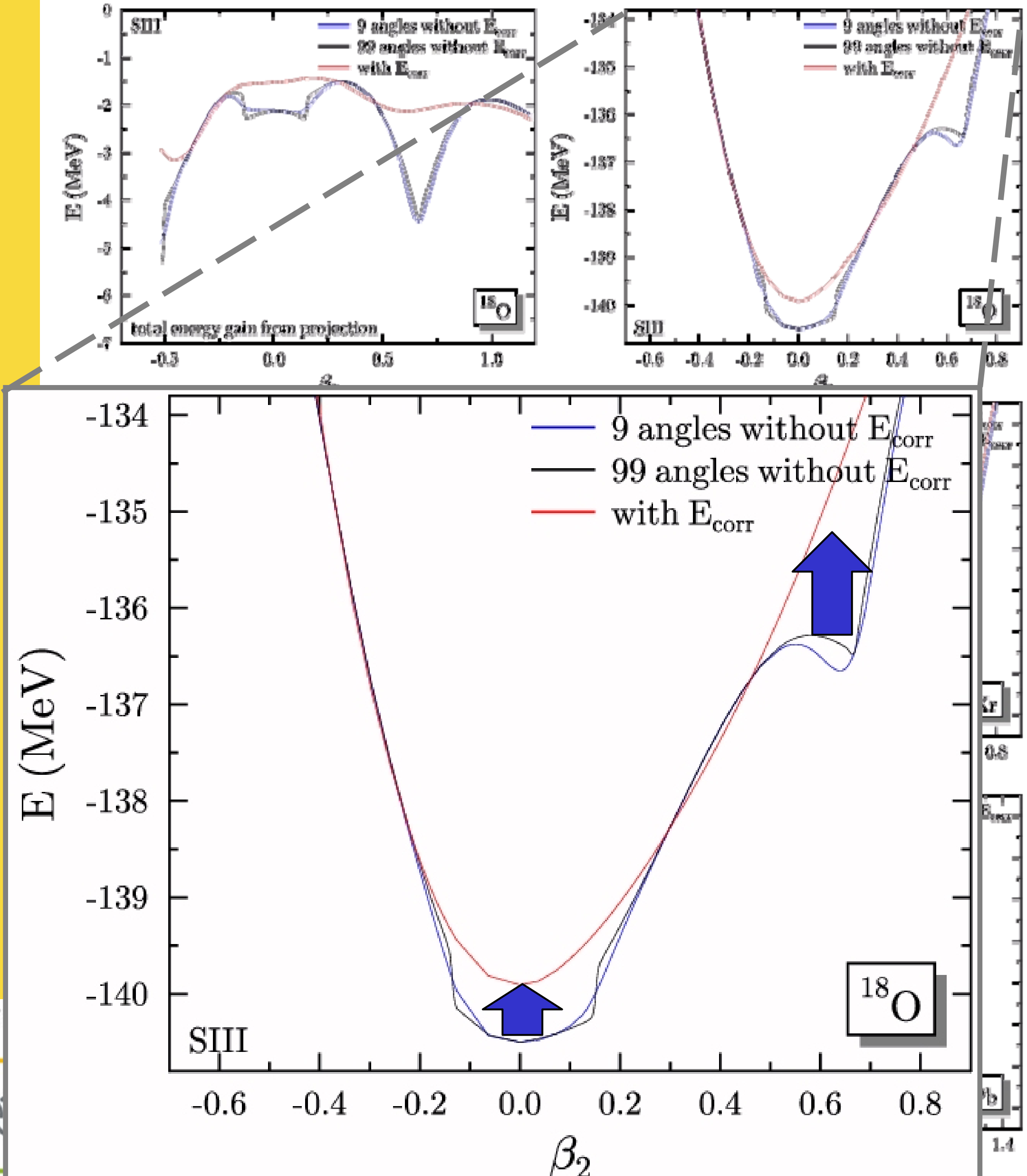
$$\mathcal{E}^{\rho\rho}_{CG}[0,\varphi] = \frac{1}{2}\sum_p \left\{ \bar{v}^{\rho\rho}_{pppp} + \bar{v}^{\rho\rho}_{\bar{p}\bar{p}\bar{p}\bar{p}} + \bar{v}^{\rho\rho}_{p\bar{p}p\bar{p}} + \bar{v}^{\rho\rho}_{\bar{p}p\bar{p}p} \right\} (u_p v_p)^4 \, \frac{(e^{2i\varphi}-1)^2}{({u_p}^2 + {v_p}^2 e^{2i\varphi})^2}$$

κκ term

$$\mathcal{E}^{\kappa\kappa}_{CG}[0,\varphi] = -\sum_p \bar{v}^{\kappa\kappa}_{p\bar{p}p\bar{p}} \, (u_p v_p)^4 \, \frac{(e^{2i\varphi}-1)^2}{({u_p}^2 + {v_p}^2 e^{2i\varphi})^2} \, ,$$

First application: particle number restoration

(II) [M. Bender, T. Duguet, D. Lacroix, to appear in PRC, arXiv:0809.2045]



- Regularized results are mesh independent
- Regularization most often reduces the gain from PNR
- Correction important at but also *away from* steps
- Correction of the order of 0.5 to 1.0 MeV
- Small enough for existing calculations to make sense
- Of the order of the required mass accuracy and spectroscopic scale
- In all cases, correction reduces the noise
- Need to study other MR modes

Conclusions

➡ Specific difficulties to be considered seriously

Dobaczewski et al, *Analysis of problem in PNR*, PRC76, 054315 (2007)

➡ Regularization method valid for any MR calculation

(I) Lacroix, et al, *General solution to pathologies*, to appear in PRC; arXiv:0809.2041

➡ Application to Particle Number Restoration

(II) Bender et al, *First application to PNR*, to appear in PRC; arXiv:0809.2045

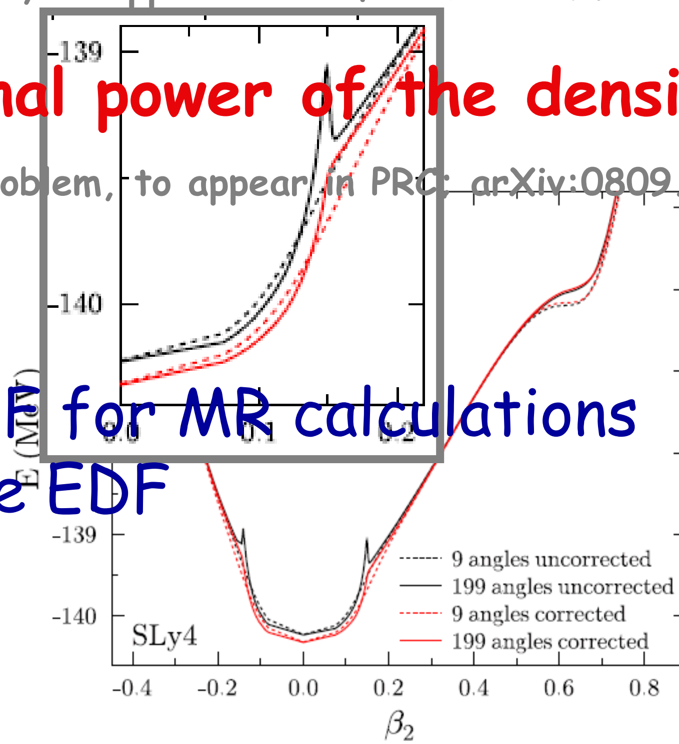
➡ **Specific case of fractional power of the density:** ρ^{γ}

(III) Duguet et al, *Non-integer powers problem*, to appear in PRC; arXiv:0809.2049

➡ Need to build

(i) Correctable EDF for MR calculations
(ii) SI- and SP-free EDF

➡ Need a constructive fran



Extra material

Addition

I TDDFT accounts for excited states

- Linear response = extended RPA
- Adiabatic approximation ⇔ Residual interaction $= \delta^2 \mathcal{E} / \delta^2\rho$
- Looks like nuclear RPA but NO feedback onto g.s. energy
- Excitation in odd nuclei include fractionation of strength

Irfu
cea
saclay

Energy Density Functional method: as practitioners use it

Basic elements

- Approaches not based on a correlated wave-function
- Energy is postulated to be a functional of one-body density (matrices) $\mathcal{E}[\rho, \kappa, \kappa^*]$
- Symmetry breaking is at the heart of the method
- Two formulations (i) Single-Reference (ii) Multi-Reference

Pros

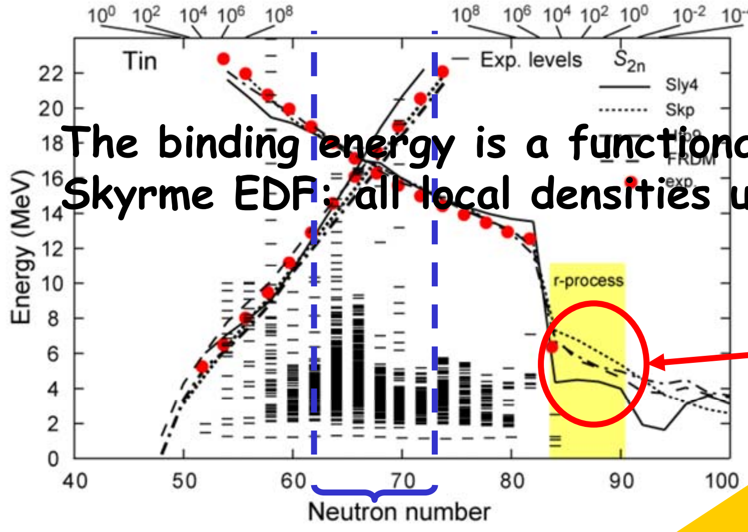
- Use of full single-particle space
- Collective picture but fully quantal
- Universality of the EDF ($A \gtrsim 16$)
- Ground-state description
- Static (smooth) correlations

Difficulties

- No universal parametrization
- Empirical $\neq$ predictive power
- Spectroscopy / odd nuclei
- Dynamical (fluctuating) correlations
- Limited accuracy ($\sigma_{2135}^{mass} \approx 700$ keV)

- Skyrme = **quasi-local** / Gogny = **non-local**
- Parameters adjusted on a set of data (bias on bulk properties so far)
- Good performances for properties of known nuclei
- "Asymptotic freedom" as one jumps into the ***next major shell***

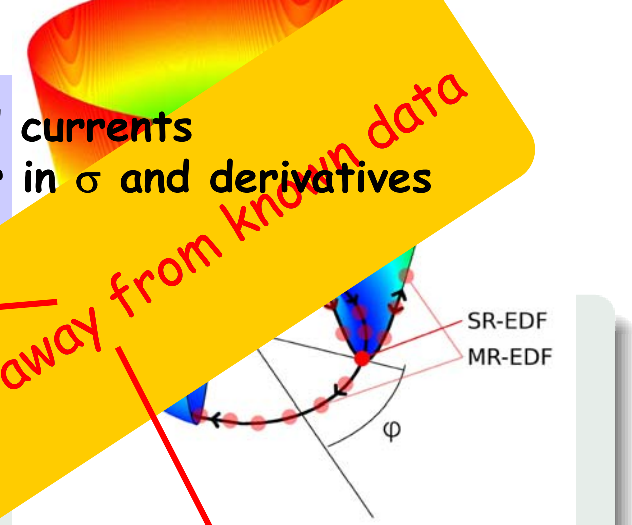
Energy Density Functionals: implementations / input



Stable isotopes

The binding energy is a functional of densities and currents

Skyrme EDF: all local densities up to second order in σ and derivatives

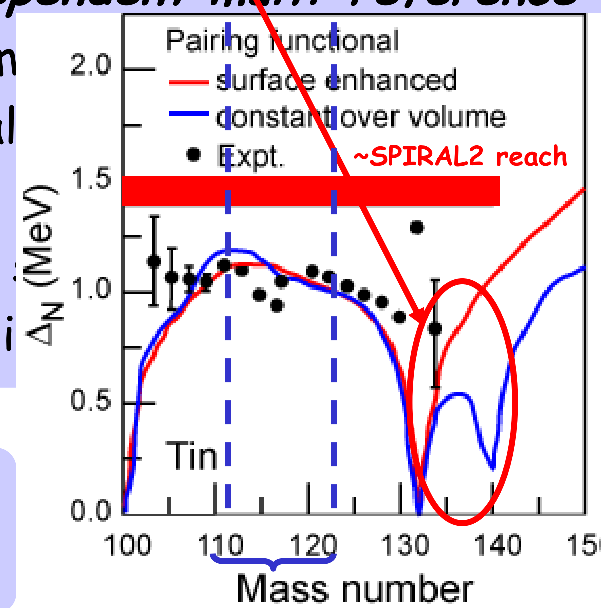


T. Duguet et al. (2006)

...ependent multi-reference

...d dynam...

- Vibrational
- Rotational
- LACM and ...
- E.M. transi...



Stable isotopes

- Good performances for known nuclei
- "Asymptotic freedom" as one goes away from known data
- Empirical = no link to NN/NNN

Couplings adjusted on a restricted set of data

Extrapolated to all other observable and nuclei

SPIRAL2 will help constrain isovector part of EDF

- In the next major shell
- Up to (N-Z)/A~0.33

- Vibrational excitations
- Reactions

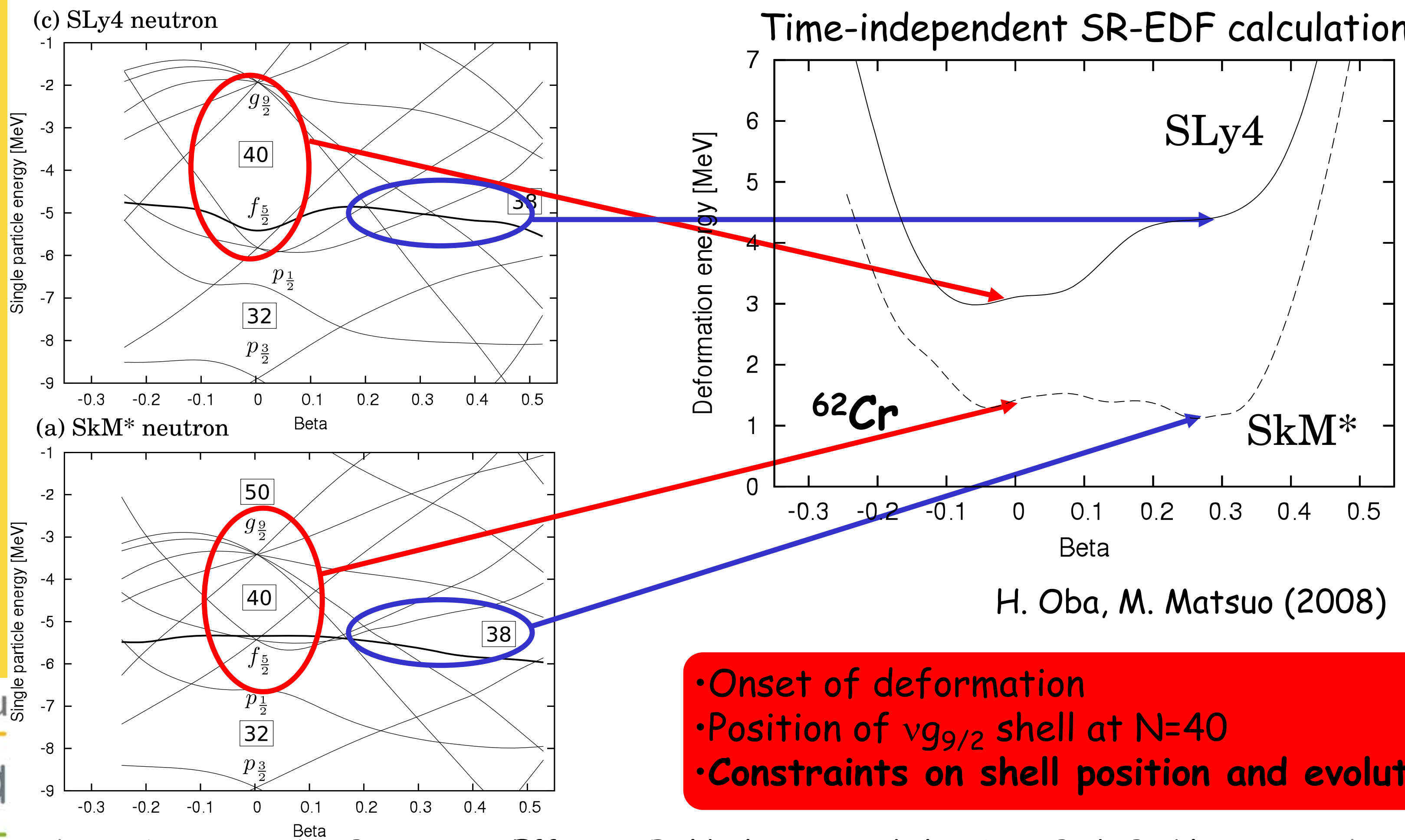
Limitations of current EDFs: one specific example

Shell evolution with N-Z

Opening and closing of shell gaps not under control

Impact the balance between spherical and deformed configurations

Weakening of N=40 shell gap in neutron-rich Cr isotopes



H. Oba, M. Matsuo (2008)

- Onset of deformation
- Position of $\nu g_{9/2}$ shell at N=40
- **Constraints on shell position and evolution**

Implementations: limitations

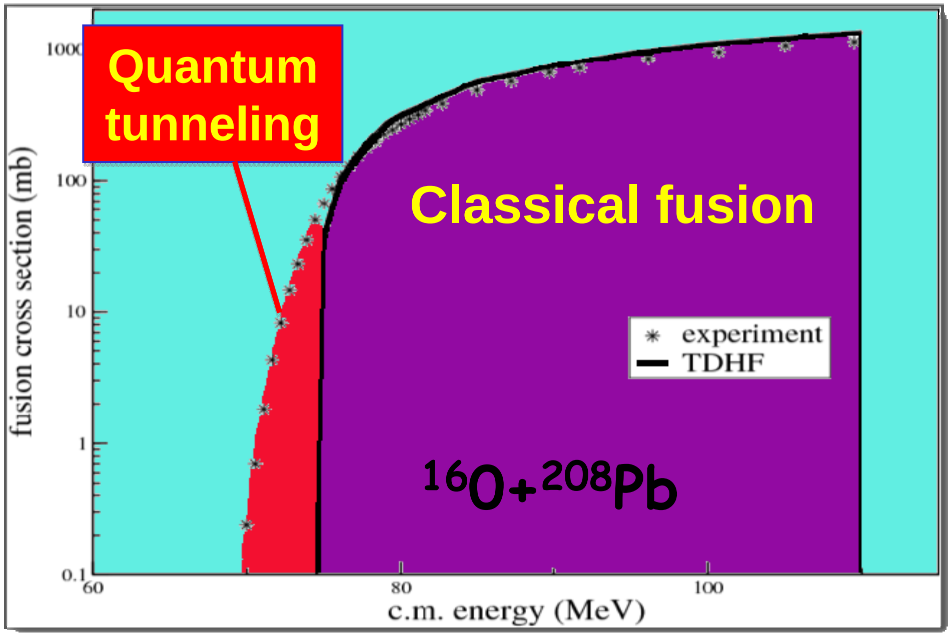
Quantum collective fluctuations in reactions
Impossibility to account for tunneling in sub-barrier fusion

Fusion cross section

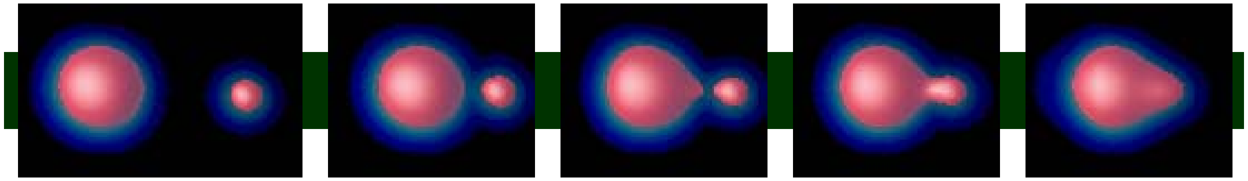
- Very satisfactory fusion barriers
- Wide range of reaction partners
- Above-threshold cross section
- **No adjustment whatsoever**

- Sub-barrier fusion
- Quantum tunneling
- **Time-dependent MR-EDF formalism**

Time-dependent SR-EDF calculation



C. Simenel (2007)



Construction of the EDF: Single-Ref.

The "nuclear physics strategy"

Hamiltonian case

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

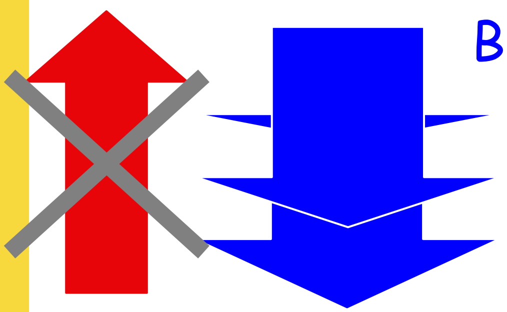
Standard Wick Theorem

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

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

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

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



Breaking the link with the Hamiltonian

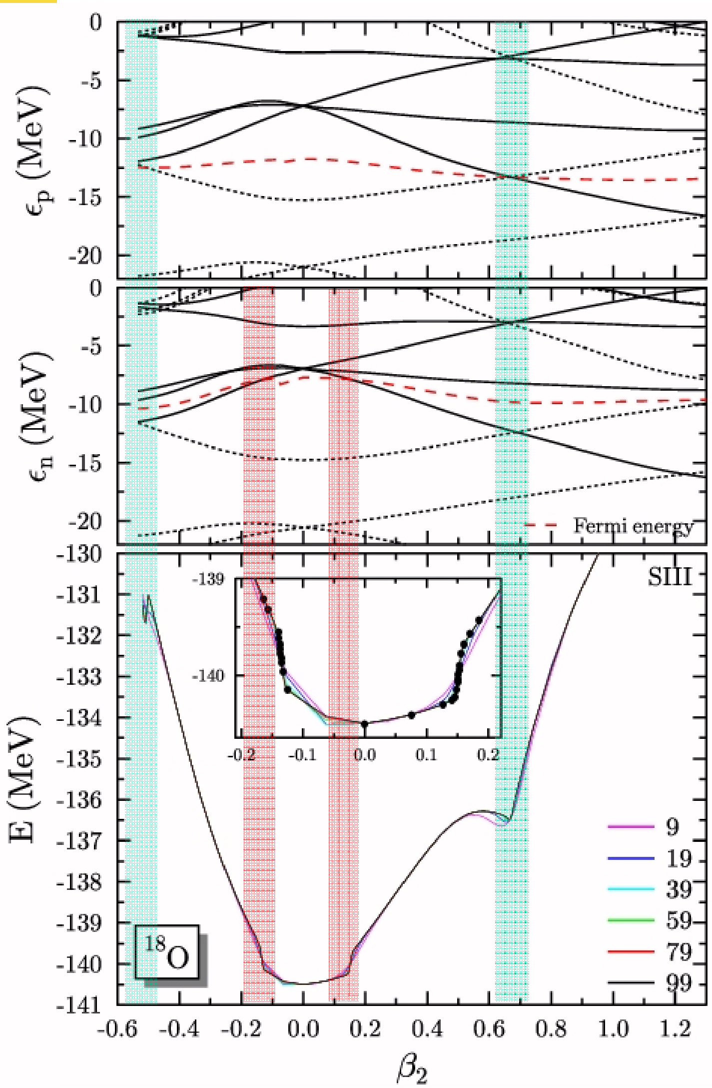
- Introduction of new terms ρ^γ
- Different interactions in ph and pp channels $\bar{v}^{\rho\rho} \neq \bar{v}^{\kappa\kappa}$
- Technical issues: coulomb, exchange…

Energy Density Functional case

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

Particle Number Restoration

(II) Bender et al, First application to PNR, arXiv/0809.2045



Trial state

$$|\Psi^N\rangle = \int_0^{2\pi} d\varphi \, \frac{e^{-i\varphi N}}{2\pi \, c_N} |\Phi_\varphi\rangle \quad \textit{with} \quad |\Phi_\varphi\rangle = e^{i\varphi \hat{N}} |\Phi_0\rangle$$

EDF calculations

$$\frac{\langle \Phi_0 | \hat{H} | \Phi_\varphi \rangle}{\langle \Phi_0 | \Phi_\varphi \rangle} \Rightarrow \mathcal{E}[0, \varphi]$$

$$\mathcal{E}^N \equiv \int_0^{2\pi} d\varphi \, \frac{e^{-i\varphi N}}{2\pi \, c_N^2} \mathcal{E}[0,\varphi] \langle \Phi_0 | \Phi_\varphi \rangle$$

Connecting states

$$|\Phi_0\rangle = \prod (u_p + v_p \, a_p^+ a_{\bar{p}}^+) |0\rangle \Rightarrow |\Phi_\varphi\rangle = \prod (u_p + v_p \, e^{2i\varphi} \, a_p^+ a_{\bar{p}}^+) |0\rangle$$

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

with

$$\bar{A}^*_{\bar{p}\bar{p}} = \bar{A}^*_{pp} = e^{-i\varphi} \left(u_p^2 + v_p^2 e^{2i\varphi} \right)$$

$$\bar{B}^*_{p\bar{p}} = -\bar{B}^*_{\bar{p}p} = u_p v_p (e^{i\varphi} - e^{-i\varphi})$$

Correction of spurious contributions

(I) Lacroix, et al, General solution to MR pathologies, arXiv/0809.2041

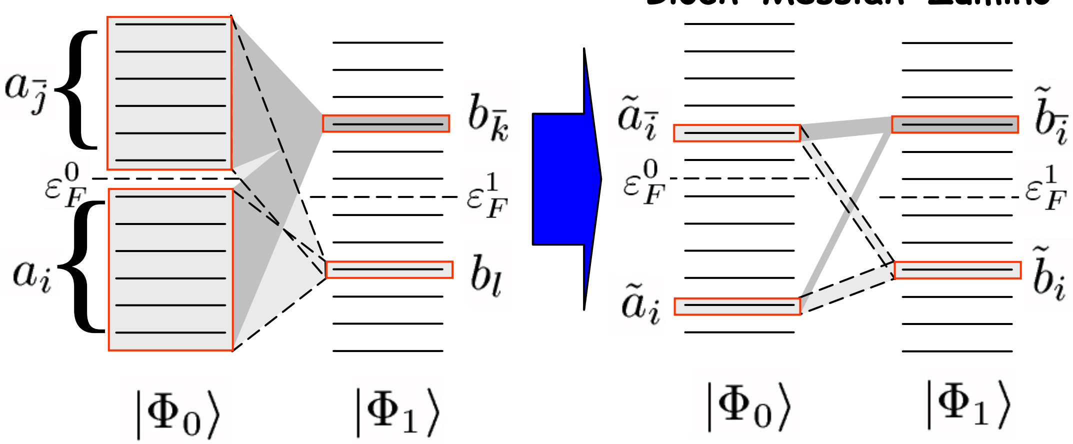
Identify problems and correct MR calculations without modifying current EDF strategy

Limited to integer power of densities (Generalization to k-body interactions)

Valid also for mixing Slater Determinants

Should correct divergences observed in Zdunczuk et al, nucl-th/0610118

Before Bloch-Messiah-Zumino | **After Bloch-Messiah-Zumino**



- *Instructive to understand BMZ Theorem*
- *Changes in numerical implementations are needed*

Illustration for Particle Number Restoration

Confirm the intuition Bender and Duguet, Int.J. Mod. Phys. E16 (2007)