Multi-reference energy density functional calculations: status, challenges, and perspectives

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Program on ”Computational and Theoretical Advances for Exotic Isotopes in the Medium Mass Region” (INT-13-1a)
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Long-term goal:

- universal microscopic model for characteristic low-lying states of nuclei . . .
- . . . and large-amplitude dynamics of nuclei . . .
- . . . irrespective of their mass and $N - Z$ . . .
- . . . their having even or odd $N$ or $Z$ . . .
- . . . using a universal effective interaction / energy density functional.

Methodology:

- Single-reference: (almost) symmetry-unrestricted self-consistent mean-fields
  ("static" deformation and pairing correlations through symmetry breaking)
- Multi-reference: symmetry restoration
- Multi-reference: configuration mixing by the Generator Coordinate Method (GCM)
  ("dynamical" deformation and pairing correlations)
Who are we?

The collaboration:

- B. Avez, B. Bally, M. Bender, J. Sadoudi
  CEN Bordeaux Gradignan, France
  formalism; beyond-mean-field models; construction of effective interactions; large-scale applications

- K. Bennaceur, D. Davesne, R. Jodon, J. Meyer
  IPN Lyon, France
  construction of effective interactions; parameter fit; nuclear matter

- T. Duguet
  SPhN / Irfu / CEA Saclay, France
  formalism; construction of effective interactions

- P.-H. Heenen, V. Hellemans, W. Ryssen
  Université Libre de Bruxelles, Belgium
  beyond-mean-field models, large-scale applications
Single-reference EDF: Some keywords

- 3d box
- at time being: triaxial symmetry
- single-reference calculations treating pairing in a Bogoliubov-type approach (”HFB”)
- constraints on quadrupole deformations and/or one component of angular momentum
- configuration constraints (”blocking”)
- Skyrme-type contact interactions + Coulomb
The standard Skyrme Energy Density Functional

\[ E_{\text{Skyrme}} = \int d^3 r \sum_{t=0,1} \left\{ C_t^\rho [\rho_0] \rho_t^2 + C_t^s [\rho_0] s_t^2 + C_t^{\Delta \rho} \rho_t \Delta \rho_t + C_t^\tau (\rho_t \tau_t - j_t^2) + C_t^T \left[ s_t \cdot T_t - \sum_{\mu,\nu=x} J_t,\mu,\nu J_t,\mu,\nu \right] + C_t^{\Delta s} s_t \cdot \Delta s_t \right. \]

\[ + C_t^F \left[ s_t \cdot F_t - \frac{1}{2} \left( \sum_{\mu=x} J_t,\mu,\mu \right)^2 - \frac{1}{2} \sum_{\mu,\nu=x} J_t,\mu,\nu J_t,\nu,\mu \right] + C_t^{\nabla s} (\nabla \cdot s_t)^2 \]

\[ \left. + C_t^{\nabla \cdot J} (\rho_t \nabla \cdot J_t + s_t \cdot \nabla \times j_t) \right\} \]

- historic link to effective Skyrme force (broken for various reasons)
- The Skyrme part of the functional is constructed such that it is invariant under time and space inversion, translation, rotation in real and isospin space, Galilei transformations etc. (otherwise projection to restore these symmetries would make no sense)
- all possible terms of 2nd order in derivatives
- density dependence (usually of velocity-independent terms only)
- blue: spherical static mean field
- blue + green: deformed static mean field
- blue + green + red: linear response / time-dependent mean field / rotating mean field / mean field of quasiparticle states / projection / GCM
Local (transition) densities and currents

\[ \rho_q(r) = \sum_{ij} \frac{\langle L|a_i^\dagger a_j|R \rangle}{\langle L|R \rangle} \psi_i^\dagger(r) \psi_j(r) \]

\[ \tau_q(r) = \sum_{ij} \frac{\langle L|a_i^\dagger a_j|R \rangle}{\langle L|R \rangle} \left[ \nabla \psi_i(r) \right]^\dagger \cdot \nabla \psi_j(r) \]

\[ J_{q,\mu\nu}(r) = -\frac{i}{2} \sum_{ij} \frac{\langle L|a_i^\dagger a_j|R \rangle}{\langle L|R \rangle} \{ \psi_i^\dagger(r) \sigma_\nu \left[ \nabla_\mu \psi_j(r) \right] - \left[ \nabla_\mu \psi_i(r) \right]^\dagger \sigma_\nu \psi_j(r) \} \]

\[ j_q(r) = -\frac{i}{2} \sum_{ij} \frac{\langle L|a_i^\dagger a_j|R \rangle}{\langle L|R \rangle} \{ \psi_i^\dagger(r) \left[ \nabla_j \psi_j(r) \right] - \left[ \nabla_j \psi_i(r) \right]^\dagger \psi_j(r) \} \]

\[ s_q(r) = \sum_{ij} \frac{\langle L|a_i^\dagger a_j|R \rangle}{\langle L|R \rangle} \psi_i^\dagger(r) \hat{\sigma} \psi_j(r) \]

\[ T_{q\mu}(r) = \sum_{ij} \frac{\langle L|a_i^\dagger a_j|R \rangle}{\langle L|R \rangle} \left[ \nabla \psi_i(r) \right]^\dagger \hat{\sigma}_\mu \cdot \left[ \nabla \psi_j(r) \right] \]

\[ F_{q,\mu}(r) = \frac{1}{2} \sum_{ij} \frac{\langle L|a_i^\dagger a_j|R \rangle}{\langle L|R \rangle} \{ \left[ \nabla \cdot \hat{\sigma} \psi_i(r) \right]^\dagger \left[ \nabla_\mu \psi_j(r) \right] + \left[ \nabla_\mu \psi_i(r) \right]^\dagger \left[ \nabla \cdot \hat{\sigma} \psi_j(r) \right] \} \]
For completeness: Other terms in the energy density functional

\[ \mathcal{E} = \mathcal{E}_{\text{kinetic}} + \mathcal{E}_{\text{Skyrme}} + \mathcal{E}_{\text{Coulomb}} + \mathcal{E}_{\text{pair}} \]

where

\[ \mathcal{E}_{\text{kinetic}} = \frac{\hbar^2}{2m} \int d^3r \, \tau(r) \]

\[ \mathcal{E}_{\text{Coulomb}} = \frac{e^2}{2} \int \int d^3r \, d^3r' \, \frac{\rho_p(r)\rho_p(r')}{|r - r'|} - \frac{3}{4} e^2 \left( \frac{3}{\pi} \right)^{1/3} \int d^3r \, \rho_p^{4/3}(r) \]

\[ \mathcal{E}_{\text{pair}} = \sum_q \int d^3r \, C^{\tilde{\rho}\tilde{\rho}}[\rho_0] \tilde{\rho}_q^*(r) \tilde{\rho}_q(r) \]

where there are two new "pairing densities"

\[ \tilde{\rho}_q(r) \equiv \sum_{ij} \frac{\langle L|a_i a_j|R\rangle}{\langle L|R\rangle} \sum_{\sigma=\pm 1} (-\sigma) \psi_i(r, -\sigma) \psi_j(r, \sigma) \]

\[ \tilde{\rho}_q^*(r) \equiv \sum_{ij} \frac{\langle L|a_i^\dagger a_j^\dagger|R\rangle}{\langle L|R\rangle} \sum_{\sigma=\pm 1} (-\sigma) \psi_i^*(r, \sigma) \psi_j^*(r, -\sigma) \]
Symmetry restoration

particle-number projector

\[ \hat{P}_{N_0} = \frac{1}{2\pi} \int_{0}^{2\pi} d\phi_N \ e^{-i\phi_N N_0} e^{i\phi_N \hat{N}} \]

angular-momentum restoration operator

\[ \hat{P}_{MK} = \frac{2J + 1}{16\pi^2} \int_{0}^{4\pi} d\alpha \int_{0}^{\pi} d\beta \sin(\beta) \int_{0}^{2\pi} d\gamma \ \mathcal{D}_{MK}^{*J}(\alpha, \beta, \gamma) \ \hat{R}(\alpha, \beta, \gamma) \]

\( K \) is the z component of angular momentum in the body-fixed frame. Projected states are given by

\[ |JMq\rangle = \sum_{K=-J}^{+J} f_J(K) \ \hat{P}_{MK} \ \hat{P}^Z \ \hat{P}^N |q\rangle = \sum_{K=-J}^{+J} f_J(K) |JMKe\rangle \]

\( f_J(K) \) is the weight of the component \( K \) and determined variationally

Axial symmetry (with the z axis as symmetry axis) allows to perform the \( \alpha \) and \( \gamma \) integrations analytically, while the sum over \( K \) collapses, \( f_J(K) \sim \delta_{K0} \)
Symmetry restoration

\[
|\text{overlap}|^2
\]

\[
E \text{(MeV)}
\]

\[
\frac{24}{\text{Mg}}
\]

\[
N
\]

\[
J
\]

\[
12^+
\]

\[
10^+
\]

\[
8^+
\]

\[
6^+
\]

\[
4^+
\]

\[
2^+
\]

\[
0^+
\]
Symmetry restoration schemes

- projection after variation (PAV): project mean-field minimum.
  - Advantage: simple
  - Problem: not variational. Unreliable in case of absent/weak static correlations

- variation after projection (VAP): vary projected state to determine the Slater determinant/HFB state that gives optimum projected state
  - Advantage: variational
  - Problem: expensive. existing codes for particle number and parity projection

- minimization after projection (MAP): generate set of mean-field states that differ in a collective coordinate that measures the amount of symmetry breaking, project them and search for the minimum of this energy curve/surface
  - Advantage: simple
  - Problem: not fully variational. Might fail if (projected) energy surface is soft in degrees of freedom that are not explicitly treated

- ... or combine projection with a mixing of states that differ in a collective coordinate that measures the amount of symmetry breaking. This automatically includes the minimum of the projected energy curve/surface and additionally correlations not related to symmetry restoration.
Configuration mixing by the symmetry-restored Generator Coordinate Method

Superposition of projected self-consistent mean-field states $|\text{MF}(q)\rangle$ differing in some collective coordinate(s) $q$

$$|NZJM_{\nu}\rangle = \sum_{q} \sum_{K=-J}^{+J} f_{j,\kappa}^{NZ}(q, K) \hat{P}_{MK}^{Z} \hat{P}^{N} |\text{MF}(q)\rangle = \sum_{q} \sum_{K=-J}^{+J} f_{j,\nu}^{NZ}(q, K) |NZ JM qK\rangle$$

with weights $f_{j,\nu}^{NZ}(q, K)$.

$$\frac{\delta}{\delta f_{j,\nu}^{*}(q, K)} \frac{\langle NZ JM_{\nu} | \hat{H} | NZ JM_{\nu}\rangle}{\langle NZ JM_{\nu} | NZ JM_{\nu}\rangle} = 0 \quad \Rightarrow \quad \text{Hill-Wheeler-Griffin equation}$$

$$\sum_{q'=-J}^{+J} \left[ \mathcal{H}_{j}^{NZ}(qK, q'K') - E_{j,\nu}^{NZ} \mathcal{I}_{j}^{NZ}(qK, q'K') \right] f_{j,\nu}^{NZ}(q'K') = 0$$

with

$$\mathcal{H}_{j}(qK, q'K') = \langle NZ JM qK | \hat{H} | NZ JM q'K' \rangle \quad \text{energy kernel}$$

$$\mathcal{I}_{j}(qK, q'K') = \langle NZ JM qK | NZ JM q'K' \rangle \quad \text{norm kernel}$$

Angular-momentum projected GCM gives the

- correlated ground state for each value of $J$
- spectrum of excited states for each $J$
Symmetry breaking and restoration

- **Benefit:** symmetries are broken on purpose: describes $np-nh$ and $p-p$ shell-model correlations ("Jahn-Teller effect", pairing, ...) with a single product state at very modest computational cost.

- **Difficulty:** scheme works only in the limits of negligible symmetry breaking and strong symmetry breaking, not in between.

- **Price to pay:** missing correlations related to symmetry restoration; difficult connection to the laboratory frame for spectroscopic observables; absence of selection rules for transitions.

- **Examples of broken symmetries:**

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<td>gauge</td>
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- **Symmetry restoration:** corresponds to fluctuations within a set of degenerate product states differing by a "rotation."
Multi-reference energy density functional methods

Multi-reference (MR) EDF is the extension of single-reference (SR) EDF analogous to GCM being an extension of HFB

◮ HF/HFB: Slater determinant/HFB state as basic building block

\[ E_{q}^{\text{HFB}} = \langle \text{SR}_q | \hat{H} | \text{SR}_q \rangle \]

◮ SR EDF: density matrices of a Slater determinant/HFB state as building blocks

\[ \mathcal{E}_q^{\text{SR}} = \mathcal{E}_q^{\text{SR}}[\rho_{qq}, \kappa_{qq}, \kappa_{qq}^*], \quad \text{where} \quad \rho_{qq} = \langle \text{SR}_q | \hat{\rho} | \text{SR}_q \rangle \quad \text{etc} \]

◮ GCM: coherent superposition of Slater determinants/HFB states

\[ |\text{MR}_\mu\rangle = \sum_q f_\mu(q) |\text{SR}_q\rangle \]

\[ \Rightarrow E_\mu = \langle \text{MR}_\mu | \hat{H} | \text{MR}_\mu \rangle = \sum_{q,q'} f_{\mu}^*(q) \langle \text{SR}_q | \hat{H} | \text{SR}_{q'} \rangle f_\mu(q') \]

◮ MR EDF: transition density matrices between a Slater determinant/HFB states as building blocks

\[ \mathcal{E}_{\mu}^{\text{MR}} = \sum_{q,q'} f_{\mu}^*(q) \mathcal{E}_{qq'}^{\text{MR}}[\rho_{qq'}, \kappa_{qq'}, \kappa_{qq'}^*] f_\mu(q') \quad \text{where} \quad \rho_{qq'} = \langle \text{SR}_q | \hat{\rho} | \text{SR}_{q'} \rangle \]
A few words on numerics: The Lagrange-mesh method

cf. the talk by Michael McNeil Forbes on monday, 8th april.

Nuclear structure codes that I am aware of using such techniques

- 2d Skyrme relativistic mean-field code by V. Blum using FFT techniques (V. Blum, Doctoral Dissertation, J. W. Goethe-Universität Frankfurt am Main, 1992)
- spherical 1d, axial 2d, 3d relativistic mean-field codes by K. Rutz using FFT techniques (K. Rutz, Doctoral Dissertation, J. W. Goethe-Universität Frankfurt am Main, 1998)
- spherical 1d, axial 2d, 3d Skyrme HF+BCS codes based on Rutz's RMF codes (M. Bender, Doctoral Dissertation, J. W. Goethe-Universität Frankfurt am Main, 1998)
Configuration mixing via the projected Generator Coordinate Method

Milestones: Spectroscopy of heavy nuclei from MR EDF


M. Bender, CEN de Bordeaux Gradignan

\begin{figure}
\centering
\includegraphics[width=\textwidth]{plot.png}
\caption{\textbf{\textit{E}} (MeV) versus $\beta_2$ for different \textit{Q}_0 (b) values.}
\end{figure}
Milestones: Spectroscopy of heavy nuclei from MR EDF

Attention: $g_i^2(q)$ is not the probability to find a mean-field state with intrinsic deformation $q$ in the collective state.
Milestones: Spectroscopy of heavy nuclei from MR EDF

$g_i^2(q)$ is not the probability to find a mean-field state with intrinsic deformation $q$ in the collective state.
in-band and out-of-band $E2$ transition moments directly in the laboratory frame with correct selection rules

- full model space of occupied particles
- only occupied single-particle states contribute to the kernels ("horizontal expansion")
- $\Rightarrow$ no effective charges necessary
- no adjustable parameters

\[
B(E2; J_{\nu}' \rightarrow J_{\nu}) = \frac{e^2}{2J' + 1} \sum_{M=-J}^{+J} \sum_{M'=-J}^{+J'} \sum_{\mu=-2}^{+2} |\langle JM\nu | \hat{Q}_{2\mu} | J' M' \nu' \rangle|^2 \\
\beta_2(t) = \frac{4\pi}{3R^2A} \sqrt{\frac{B(E2; J \rightarrow J - 2)}{(J020 |(J-2)0)^2 e^2}} \quad \text{with} \quad R = 1.2 A^{1/3}
\]
Static and Dynamic Quadrupole Correlation Energies


M. Bender, CEN de Bordeaux Gradignan

MREDF
Intrinsic Deformation and Quadrupole Correlation Energy

Eigenvalues of the single-particle Hamiltonian vs. $S_{2q}$

lower panel: $-S_{2p}(Z=50, N)/2$

The global linear trend is taken out subtracting

\[ \frac{N-82}{2} [S_{2p}(Z=50, N=50) - S_{2p}(Z=50, N=82)] \]

using the spherical mean-field $S_{2p}$


lower panel: $-S_{2n}(Z, N=50)/2$

The global linear trend is taken out subtracting

\[ \frac{N-50}{2} [S_{2n}(Z=28, N=50) - S_{2n}(Z=50, N=50)] \]

using the spherical mean-field $S_{2n}$
Eigenvalues of the single-particle Hamiltonian vs. $S_{2q}$

lower panel: $-S_{2p}(Z=50, N)/2$

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$$\frac{N-82}{2} \left[ S_{2p}(Z=50, N=50) - S_{2p}(Z=50, N=82) \right]$$

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The global linear trend is taken out subtracting $\frac{N-82}{2}[S_{2p}(Z=50, N=50) - S_{2p}(Z=50, N=82)]$ using the spherical mean-field $S_{2p}$
Milestones: Angular momentum projection of triaxial states

\[ J = 0 \text{ projected deformation energy surface} \]

Solving the sign problem in MR EDF

Overlap from Pfaffian formula, Benoît Avez & M. B., PRC 85 (2012) 034255

$\alpha, \beta$ held fixed at some values, $\gamma$ varied

lowest blocked one-quasiparticle state in $^{25}\text{Mg}$

$^{24}\text{Mg}$ cranked to $I = 8\hbar$

New developments: use angular-momentum optimized states

Limitations of the existing implementations of the method
- limited to even-even nuclei
- collective states only
- excitation spectra too spread out

What is the missing physics?
- explicit coupling to single-particle degrees of freedom

How to introduce the missing physics?
- Use HFB states breaking intrinsic time-reversal invariance as basis states for the projected GCM
- cranked HFB states describe the alignment of single-particle states with the rotation axis and the weakening of pairing with increasing $J$
- blocked HFB states describe single-particle excitations ($K$ isomers in even-even nuclei, odd-$A$ nuclei, odd-odd nuclei)

+ adjustment of improved energy functionals
Problems ...

- pure particle-number projection
Problems ...

- pure particle-number projection
- First analysis in a strict energy density functional framework and of EDF-specific consequences by Dobaczewski, Stoitsov, Nazarewicz, Reinhard, PRC 76 (2007) 054315
All standard energy density functionals (EDF) used for mean-field models and beyond do not correspond to the expectation value of a Hamiltonian for at least one of the following reasons:

- density dependences
- the use of different effective interactions in the particle-hole and pairing parts of the energy functional
- the omission, approximation or modification of specific exchange terms that are all introduced for phenomenological reasons and/or the sake of numerical efficiency.

Consequence: breaking of the exchange symmetry under particle exchange when calculating the energy, leading to non-physical interactions of a given nucleon or pair of nucleons with itself.

These self-interactions remain (usually) hidden in the mean field.

In the extension to symmetry-restored GCM, these terms cause

- discontinuities and divergences in symmetry-restored energy surfaces
- breaking of sum rules in symmetry restoration
- potentially multi-valued EDF in case of standard density-dependencies
What to do?

1. constructing the EDF as expectation value of a strict Hamiltonian. New problem: numerically very costly due to Coulomb exchange & pairing; no available parameterizations of high quality (the difficulties to construct such parametrizations was the main motivation to use EDFs in the 1970s).

2. construct the EDF from a density-dependent Hamiltonians with special treatment of the density entering density dependent terms for which numerically efficient high-quality parameterizations can be easily constructed. Problem: numerically very costly due to Coulomb exchange & pairing; cannot be defined for all possible configuration mixing [Robledo, J. Phys. G 37 (2010) 064020].

3. introducing a regularization scheme of the EDF that allows for the use of (almost) standard functionals [Lacroix, Duguet, & Bender, PRC 79 (2009) 044318] for which numerically efficient high-quality parameterizations can be easily constructed [Washiyama, Bennaceur, Avez, Bender, Heenen, & Hellemans, PRC 86 (2012) 054309]. Problem: complicated formalism.

We tried the last option first.
The regularisation: it *almost* works

Usual number of Euler and gauge angles:

M. B., B. Avez, T. Duguet, P.-H. Heenen, D. Lacroix, unpublished
The regularisation: it *almost* works

Usual number of Euler and ridiculously large number of gauge angles:

⇒ dependence on the discretization that becomes visible only when using unreasonably fine discretizations
spectra projected from cranked states are (almost) realistic only when regularising
improved moment of inertia at low spin
reproduction of backbending requires scanning the whole energy surface

B. Avez, B. Bally, M. B., P.-H. Heenen, unpublished
All states are constructed as blocked one-quasiparticle HFB states
The regularization can become large

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</tbody>
</table>

B. Bally, B. Avez, M. B., P.-H. Heenen, unpublished
There are remaining problems

- Non-convergence of combined $N$ and $J$ projection (on a very small scale, though)
- Non-diagonal regularized MR EDF kernels can be decomposed on unphysical particle numbers (i.e. components that have strictly zero norm), including negative particle numbers
- Small components (still) take unphysical values when regularising which can be demonstrated using a cranking constraint to control the size of $K = 1$ components
- Impossibility to perform $K$ mixing in a controlled manner
Again: What to do?

1. constructing the EDF as expectation value of a strict Hamiltonian. New problem: numerically very costly due to Coulomb exchange & pairing; no available parameterizations of high quality (the difficulties to construct such parametrizations was the main motivation to use EDFs in the 1970s).

2. construct the EDF from a density-dependent Hamiltonians with special treatment of the density entering density dependent terms for which numerically efficient high-quality parameterizations can be easily constructed. Problem: numerically very costly due to Coulomb exchange & pairing; cannot be defined for all possible configuration mixing [Robledo, J. Phys. G 37 (2010) 064020].

3. introducing a regularization scheme of the EDF that allows for the use of (almost) standard functionals [Lacroix, Duguet, & Bender, PRC 79 (2009) 044318] for which numerically efficient high-quality parameterizations can be easily constructed [Washiyama, Bennaceur, Avez, Bender, Heenen, & Hellemans, PRC 86 (2012) 054309]. Problem: complicated formalism.

At last, we try the first option.
How to construct a suitable Hamiltonian?

- We need a Skyrme Hamiltonian (without density dependence)
- there no existing parametrization that gives simultaneously
  - realistic "standard" nuclear matter properties
  - repulsive spin-spin interaction
  - attractive pairing

which was the reason to introduce density dependences etc. in the 1970s.

First try: SLyMR0

\[ \hat{v} = t_0 \left( 1 + x_0 \hat{P}_{\sigma} \right) \hat{\delta}_{\mathbf{r}_1 \mathbf{r}_2} + \frac{t_1}{2} \left( 1 + x_1 \hat{P}_{\sigma} \right) \left( \mathbf{k}_{12}^2 \hat{\delta}_{\mathbf{r}_1 \mathbf{r}_2} + \hat{\delta}_{\mathbf{r}_1 \mathbf{r}_2} \mathbf{k}_{12}^2 \right) + t_2 \left( 1 + x_2 \hat{P}_{\sigma} \right) \mathbf{k}_{12}' \cdot \hat{\delta}_{\mathbf{r}_1 \mathbf{r}_2} \mathbf{k}_{12}' + i W_0 \left( \hat{\sigma}_1 + \hat{\sigma}_2 \right) \cdot \mathbf{k}_{12}' \times \hat{\delta}_{\mathbf{r}_1 \mathbf{r}_2} \mathbf{k}_{12}' + u_0 \left( \hat{\delta}_{\mathbf{r}_1 \mathbf{r}_3} \hat{\delta}_{\mathbf{r}_2 \mathbf{r}_3} + \hat{\delta}_{\mathbf{r}_3 \mathbf{r}_2} \hat{\delta}_{\mathbf{r}_1 \mathbf{r}_2} + \hat{\delta}_{\mathbf{r}_2 \mathbf{r}_1} \hat{\delta}_{\mathbf{r}_3 \mathbf{r}_1} \right) + v_0 \left( \hat{\delta}_{\mathbf{r}_1 \mathbf{r}_3} \hat{\delta}_{\mathbf{r}_2 \mathbf{r}_3} \hat{\delta}_{\mathbf{r}_3 \mathbf{r}_4} + \hat{\delta}_{\mathbf{r}_1 \mathbf{r}_2} \hat{\delta}_{\mathbf{r}_3 \mathbf{r}_2} \hat{\delta}_{\mathbf{r}_2 \mathbf{r}_4} + \cdots \right) \]

J. Sadoudi, M. Bender, K. Bennaceur, D. Davesne, R. Jodon, and T. Duguet, Physica Scripta T, in press
First try: standard two-body + contact 3-body + contact 4-body

- it is impossible to fulfil the usual nuclear matter constraints, to have stable interactions and attractive pairing
- no "best fit" possible
- very bad performance compared to standard functionals

J. Sadoudi, M. Bender, K. Bennaceur, D. Davesne, R. Jodon, and T. Duguet, Physica Scripta, in press
MR EDF based on cranked HFB states: The example of $^{24}\text{Mg}$

$^{24}\text{Mg}$

$\Rightarrow$ SLyMR0 is not completely disastrous for the description of this phenomenon  
$\Rightarrow$ deformation of HF and HFB+LN is very different for SLyMR0
Decomposition of states

cranked HF ground state

cranked HFB+LN ground state

HF $K = 8$ state
Decomposition

\[ K=8 \]

\[ 8^+ \]

\[ E (\text{MeV}) \]

\[ \begin{array}{c}
17 \\
16 \\
15 \\
14 \\
13 \\
12 \\
11 \\
10 \\
9 \\
8 \\
7 \\
6 \\
5 \\
4 \\
3 \\
2 \\
1 \\
0 \\
\end{array} \]

\[ 10^+ \quad 10^+ \]

\[ 8^+ \]

\[ 8^+ \quad 8^+ \]

\[ 6^+ \]

\[ 6^+ \quad 6^+ \]

\[ 4^+ \quad 4^+ \]

\[ 2^+ \quad 2^+ \]

\[ \text{cranked} \]

\[ \text{projected} \]

\[ \text{SLyMR0} \]

\[ \begin{array}{c}
\text{HF} \\
\text{HFB+LN} \\
\text{HF, I}=0 \\
\text{HF, lowest} \\
\end{array} \]

\[ 24\text{Mg} \]

\[ 8^+ \]

\[ 8^+ \]

\[ 4^+ \]

\[ 2^+ \quad 0^+ \]

\[ 6^+ \quad 4^+ \quad 2^+ \]

\[ 155 \quad 149 \quad 160 \quad 5 \quad 239 \quad 8 \]

\[ 2^+ \]

\[ 0^+ \quad 88 \quad 10 \quad 15 \]

\[ \text{Expt.} \]
$\beta = 0.62, \gamma = 14.9^\circ$

$\langle I_x \rangle = 0$  

$\langle I_x \rangle = \sqrt{J(J+1)}$

experiment
Energy surfaces

\begin{align*}
\text{PNR only } & \quad {}^{24}\text{Mg} \\
\text{PNR+AMR } & \quad {}^{24}\text{Mg} \\
\end{align*}

\begin{align*}
E \text{ [MeV]} & = 20.0 \\
& \text{[Color Bar]} \\
\end{align*}

\begin{align*}
\beta & = 0.0 \\
& \to 1.4 \\
\gamma \text{ [deg]} & = 0 \\
& \to 90 \\
\end{align*}

PRELIMINARY
Odd-$A$ nuclei with SLyMR0: The example of $^{25}$Mg

"False vacuum" (non-blocked HFB ground state with $\langle \hat{N} \rangle = 13, \langle \hat{Z} \rangle = 12$)

B. Bally, B. Avez, M. B., P.-H. Heenen (to be published)

Blocked HFB 1-quasiparticle state, where blocked particle has $\langle j_z \rangle \approx 5/2$
First ”beyond-mean-field” results for odd-$A$ nuclei with SLyMR0

Blocked 1-qp state with $\langle j_z \rangle \approx 5/2$, projected on $Z = 12$, $N = 13$, $J = 5/2^+$.  

Blocked 1-qqp state with $\langle j_z \rangle \approx 3/2$, projected on $Z = 12$, $N = 13$, $J = 3/2^+$.  

Decomposition of the blocked HFB 1-quasiparticle state that gives the lowest energy after projection.  

Full GCM of projected states.
Ongoing improvements: 3-body terms of 2nd order in gradients

- most general central 3-body force has been constructed by J. Sadoudi with a dedicated formal algebra code

\[
\hat{v}_{123} = u_0 \left( \hat{\delta}_{r_1 r_3} \hat{\delta}_{r_2 r_3} + \hat{\delta}_{r_3 r_2} \hat{\delta}_{r_1 r_2} + \hat{\delta}_{r_2 r_1} \hat{\delta}_{r_3 r_1} \right) \\
+ \frac{u_1}{2} \left[ 1 + y_1 P_{12}^\sigma \right] \left( \hat{k}_{12} \cdot \hat{k}_{12} + \hat{k}'_{12} \cdot \hat{k}'_{12} \right) \hat{\delta}_{r_1 r_3} \hat{\delta}_{r_2 r_3} \\
+ \frac{u_1}{2} \left[ 1 + y_1 P_{31}^\sigma \right] \left( \hat{k}_{31} \cdot \hat{k}_{31} + \hat{k}'_{31} \cdot \hat{k}'_{31} \right) \hat{\delta}_{r_3 r_2} \hat{\delta}_{r_1 r_2} \\
+ \frac{u_1}{2} \left[ 1 + y_1 P_{23}^\sigma \right] \left( \hat{k}_{23} \cdot \hat{k}_{23} + \hat{k}'_{23} \cdot \hat{k}'_{23} \right) \hat{\delta}_{r_2 r_1} \hat{\delta}_{r_3 r_1} \\
+ u_2 \left[ 1 + y_21 P_{12}^\sigma + y_22 \left( P_{13}^\sigma + P_{23}^\sigma \right) \right] \left( \hat{k}_{12} \cdot \hat{k}'_{12} \right) \hat{\delta}_{r_1 r_3} \hat{\delta}_{r_2 r_3} \\
+ u_2 \left[ 1 + y_21 P_{31}^\sigma + y_22 \left( P_{32}^\sigma + P_{12}^\sigma \right) \right] \left( \hat{k}_{31} \cdot \hat{k}'_{31} \right) \hat{\delta}_{r_3 r_2} \hat{\delta}_{r_1 r_2} \\
+ u_2 \left[ 1 + y_21 P_{23}^\sigma + y_22 \left( P_{21}^\sigma + P_{31}^\sigma \right) \right] \left( \hat{k}_{23} \cdot \hat{k}'_{23} \right) \hat{\delta}_{r_2 r_1} \hat{\delta}_{r_3 r_1}
\]

- complete functional in particle-hole and $T = 1$ pairing channel
- derivation of nuclear matter properties
- derivation of mean fields and pairing fields
- implementation in spherical HFB code
- first preliminary fits
Take-away messages

- Generalization of MR EDF to angular-momentum-optimized reference states
  - improved moments of inertia
  - $K$ isomers
  - odd-$A$ nuclei
- At time being, there is no scheme to safely handle general EDFs in multi-reference framework. When conserving many symmetries on the single-reference level, there are two recipes that more-or-less almost work
  - density-dependent Hamiltonians with special treatment of the density entering the density dependence
  - regularized MR EDF

Both require particular forms of the EDF.

- Going back to Hamiltonians is (at time being) the safest strategy to follow. This shifts the problem from constructing a consistent MR EDF framework for general functionals to constructing treatable and performant pseudo-potentials.

Publications are in preparation.