Beyond-mean-field calculations based on time-reversal-invariance-breaking HFB states — prospects and perspectives

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work begun while having been at the

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Université Claude Bernard Lyon 1

What is meant by "beyond-mean-field calculation" during this talk

beyond mean field $\Leftrightarrow$ configuration mixing based on symmetry-restored symmetry-breaking states

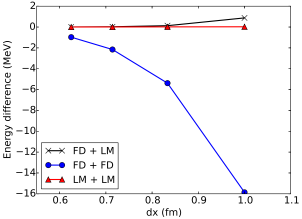
- generate a set of (deformed and/or otherwise symmetry breaking) HFB states with suitable constraints on shape and/or other degrees of freedom. (here: time-reversal breaking states conserving only $\hat{P}$, $\hat{R}_x$ and $\hat{S}_y^T$, only like-particle pairing)
- restore the broken symmetries by projection on good quantum numbers. (here: Z, N, J^2, J_z)
- mix the (non-orthogonal) states projected on the same set of quantum numbers by solving a generalized eigenvalue problem, usually called Hill-Wheeler-Griffin (HWG) equation in this context.

What is needed:

- a HFB solver generating the symmetry-breaking states.
- a code calculating projected many-body matrix elements.
- a HWG solver.
- an effective interaction.

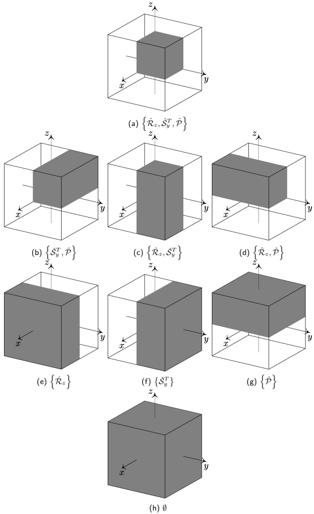
MOCCa: a new flexible HFB solver using coordinate-space representation

- coordinate space representation
- flexible description of shapes of the density and the current distribution. At present, any subgroup out of $\hat{P}$, $\hat{R}_x$, $\hat{S}_y^T$, and $\hat{T}$ is possible.
- high numerical precision obtained with Lagrange-mesh techniques



Ryssens, Heenen, and Bender, PRC 92 (2015) 064318

- multiple constraints on the shape of densities and currents.
- HFB.



W. Ryssens, Ph.D. thesis (Université Libre de Bruxelles, 2016).

Construction of effective interactions with better performance

- better *local* control of single-particle structure is possible, . . .

  Shi, Dobaczewski, Greenlees, PRC 89 (2014) 034309

  . . . but better *global* control of single-particle structure is difficult

  Lesinski, Bender, Bennaceur, Duguet, Meyer, PRC 76 (2007) 014312

  Bender, Bennaceur, Duguet, Heenen, Lesinski, Meyer, PRC 80 (2009) 064302

  Kortelainen, Dobaczewski, Mizuyama, Toivanen, PRC 77 (2008) 064307

  Kortelainen, McDonnell, Nazarewicz, Olsen, Reinhard, Sarich, Schunck, Wild, Davesne, Erler, Pastore, PRC 89 (2014) 054314

- better control of surface properties

  Kortelainen, McDonnell, Nazarewicz, Reinhard, Sarich, Schunck, Stoitsov, Wild, PRC 85 (2012) 024304

  Jodon, Bennaceur, Meyer, Bender, PRC 94 (2016) 024335.

- better control of symmetry energy

  Li, Ramos, Verde, Vidaña [edts], Topical Issue on "Nuclear Symmetry Energy", EPJA 50 (2014)

- better control of response properties
- suppression of spurious instabilities

  Hellemans, Pastore, Duguet, Bennaceur, Davesne, Meyer, Bender, Heenen, PRC 88 (2013) 064323

  Pastore, Davesne, Bennaceur, Meyer, Hellemans, Phys Scr T154 (2013) 014014

Construction of new forms of effective interactions

- Skyrme-type interactions with higher-order terms in derivatives

  Carlsson, Dobaczewski, Kortelainen, PRC 78 (2008) 044326

  Raimondi, Carlsson, Dobaczewski, PRC 83 (2011) 054311

  Davesne, Pastore, Navarro, JPG 40 (2013) 095104

  Becker, Davesne, Meyer, Pastore, Navarro, JPG 42 (2015) 034001

- Skyrme-type interactions with three-body interactions with gradients

  Sadoudi, thèse, Université de Paris-Sud XI (2011)

  Sadoudi, Duguet, Meyer, Bender, PRC 88 (2013) 064326

  Jodon, thèse, Université Lyon I (2014)

- finite-range density dependences

  Chappert, Pillet, Girod, Berger, PRC 91 (2015) 034312

- regularised contact interactions (combining Gaussians à la Gogny with gradients à la Skyrme)

  Raimondi, Bennaceur, Dobaczewski, JPG 41 (2014) 055112

- non-local three-body forces simulating density dependences

  Gezerlis, Bertsch, PRL 105 (2010) 212501

  Lacroix, Bennaceur, PRC 91 (2015) 011302(R)

- or try a different strategy: explicit in-medium correlations from MBPT

  Duguet, Bender, Ebran, Lesinski, Somà, EPJA 51 (2015) 162

Two features of existing effective interactions that might cause problems:

1. violation of Pauli principle when setting up the EDF
2. non-analytical density dependence of coupling constants

Anguiano, Egido, Robledo, NPA696 (2001) 467

Dobaczewski, Stoitsov, Nazarewicz, Reinhard, PRC76 (2007) 054315

Lacroix Duguet, Bender, *et al* Phys. Rev. C 79 (2009) 044318, 044319, and 044320

Strategies how to cope with them:

- Ignore and continue to run calculations.
- Stop using MR techniques and live happily running SR calculations.
- Regularize EDF with a physics-motivated regularization (Lacroix *et al*). Works for particle-number projections, fails for spatial symmetries.
- Regularize EDF with a mathematics-motivated regularization (Satuła and Dobaczewski). Unclear if implementable into all numerical representations.
- Use a density-dependent effective interaction and limit yourself to expressions for density-dependent coupling constants that remain integrable. Constrains form of density dependence and might limit possible applications.
- Construct pseudo-potential based EDFs (i.e. EDFs that are the expectation value of a Hamiltonian with density-*in*dependent coupling constants.
- Construct pseudo-potential based EDF and calculate the physics at the origin of density dependences explicitly.

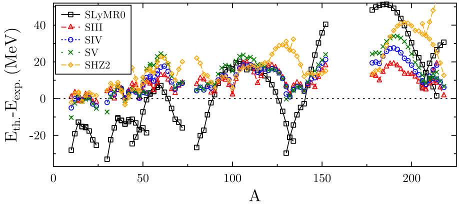
Pseudo-potentials for MR EDF. First try: SLyMR0

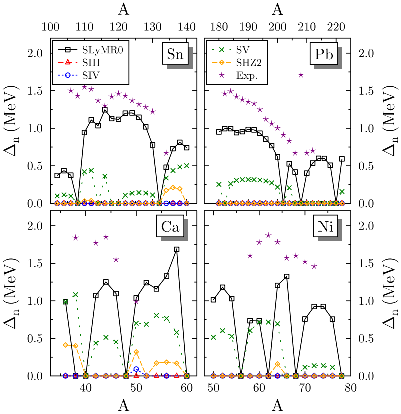
First try: SLyMR0 (= "SV" + gradientless 3-body and 4-body forces)

$$
\begin{aligned}
\hat{v} = {} & t_0 \left(1 + x_0 \hat{P}_\sigma\right) \hat{\delta}_{r_1 r_2} \\
& + \frac{t_1}{2} \left(1 + x_1 \hat{P}_\sigma\right) \left(\hat{\mathbf{k}}_{12}^{\prime\,2} \hat{\delta}_{r_1 r_2} + \hat{\delta}_{r_1 r_2} \hat{\mathbf{k}}_{12}^{2}\right) \\
& + t_2 \left(1 + x_2 \hat{P}_\sigma\right) \hat{\mathbf{k}}_{12}^{\prime} \cdot \hat{\delta}_{r_1 r_2} \hat{\mathbf{k}}_{12} \\
& + \mathrm{i}\, W_0 \left(\hat{\boldsymbol{\sigma}}_1 + \hat{\boldsymbol{\sigma}}_2\right) \cdot \hat{\mathbf{k}}_{12}^{\prime} \times \hat{\delta}_{r_1 r_2} \hat{\mathbf{k}}_{12} \\
& + u_0 \left(\hat{\delta}_{r_1 r_3} \hat{\delta}_{r_2 r_3} + \hat{\delta}_{r_3 r_2} \hat{\delta}_{r_1 r_2} + \hat{\delta}_{r_2 r_1} \hat{\delta}_{r_3 r_1}\right) \\
& + v_0 \left(\hat{\delta}_{r_1 r_3} \hat{\delta}_{r_2 r_3} \hat{\delta}_{r_3 r_4} + \hat{\delta}_{r_1 r_2} \hat{\delta}_{r_3 r_2} \hat{\delta}_{r_2 r_4} + \cdots\right)
\end{aligned}
$$

Sadoudi, Bender, Bennaceur, Davesne, Jodon, Duguet, Physica Scripta T154 (2013) 014013

Pseudo-potentials for MR EDF. First try: SLyMR0

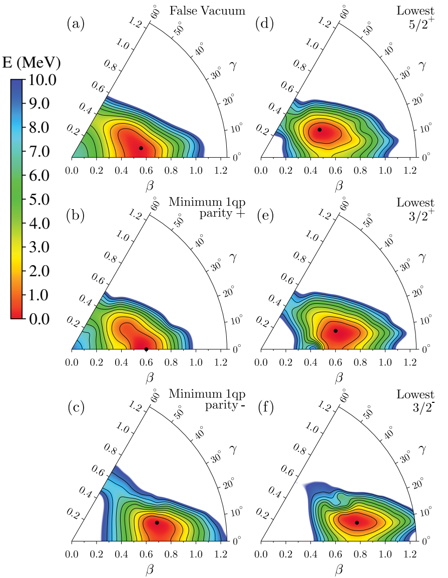




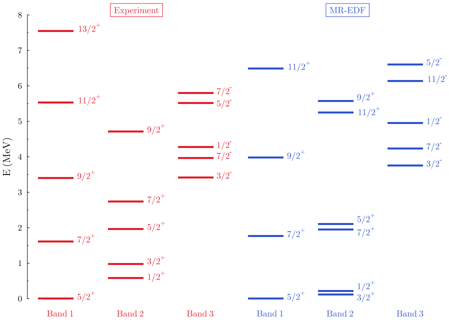
- it is impossible to fullfil the usual nuclear matter constraints , to have stable interactions and attractive pairing
- no "best fit" possible
- very bad performance compared to standard general functionals

Sadoudi, Bender, Bennaceur, Davesne, Jodon, and Duguet, Physica Scripta T154 (2013) 014013

Proof-of-principle: Symmetry-restored GCM for ^{25}Mg



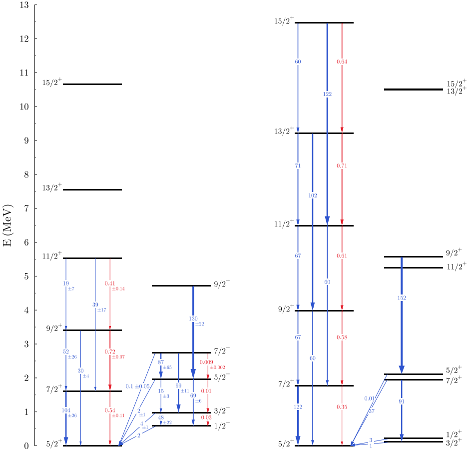
Angular-momentum and particle-number projected GCM of blocked triaxial one-quasiparticle states



B. Bally, doctoral thesis, Université de Bordeaux (2014)

Bally, Avez, Bender, Heenen, PRL 113 (2014) 162501

Proof-of-principle: Symmetry-restored GCM for ^{25}Mg

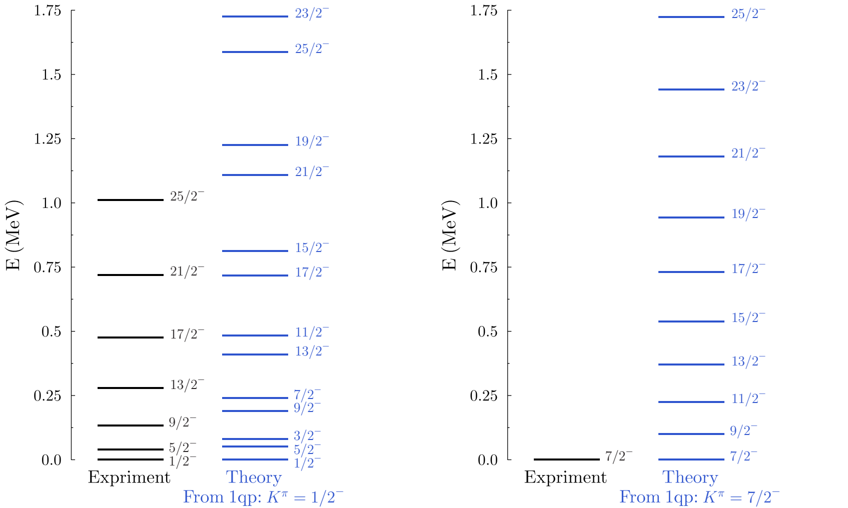


- spectroscopic quadrupole moment Q_s of the $5/2^+$ ground state:
  Exp: 20.1 ± 0.3 e fm^2
  Calc: 23.25 e fm^2
- magnetic moment μ of the $5/2^+$ ground state in nuclear magnetons:
  Exp: -0.855
  Calc: -1.054

Bally, Avez, Bender, Heenen, PRL 113 (2014) 162501

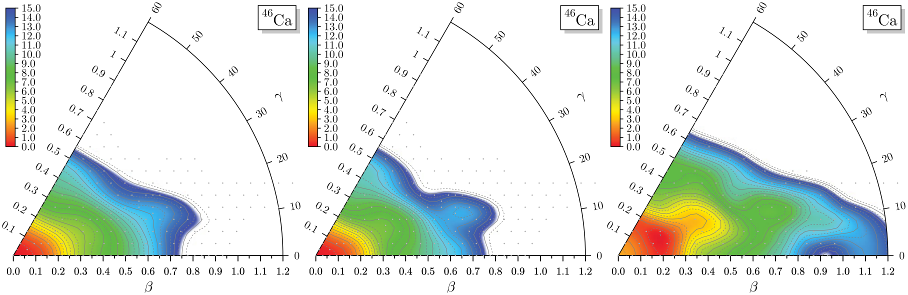
Data from Nuclear Data Sheets 110 (2009) 1691

Proof-of-principle: Symmetry-restoration for ^{251}Md



Bally, Bender, Heenen, unpublished

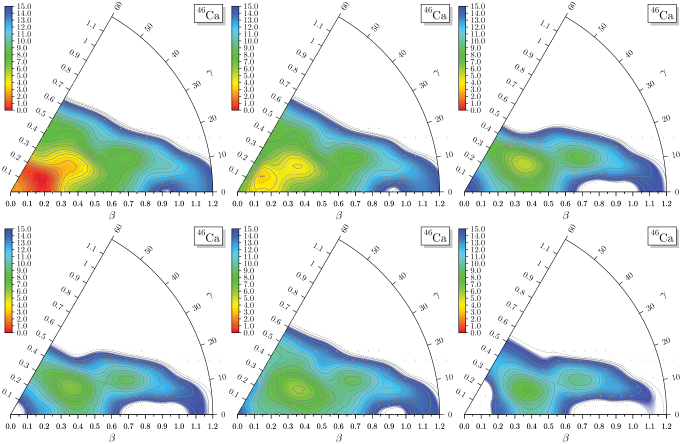
Low-lying states in ^{46}Ca



Left: Non-projected total energy of the HFB vacua (without LN correction) relative to the spherical configuration. Middle: $N = 26$, $Z = 20$ projected total energy of the HFB vacua relative to the spherical configuration. Right: Energy of the projected $N = 26$, $Z = 20$, $J = 0$ HFB vacua.

Bender& Heenen to be published

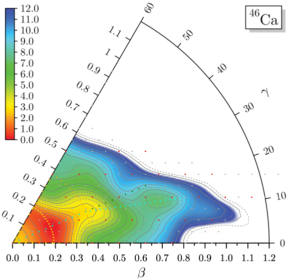
Low-lying states in ^{46}Ca

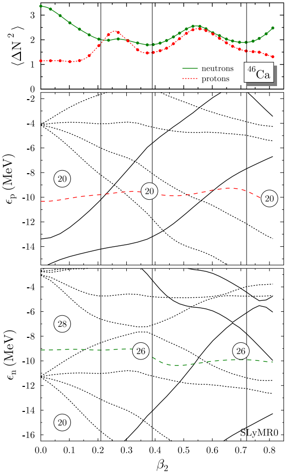


Top row: Right: Energy of the $J = 0$ HFB vacua. Middle: Energy of the lowest K-mixed $J = 2$ projected state . Right: Energy of the second K-mixed $J = 2$ state . Bottom row: Right: Energy of the $J = 3$ state. Middle: Energy of the lowest K-mixed $J = 4$ projected state. Right: Energy of the second K-mixed $J = 4$ state. The total energy is relative to the minimum of the $J = 0$ energy surface. All states are projected on $N = 26$, $Z = 20$,

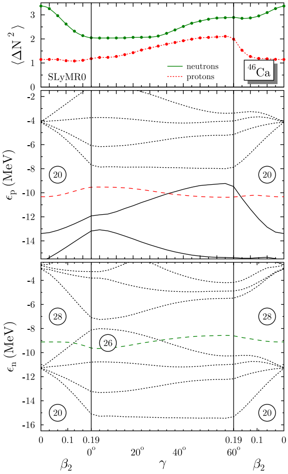
Bender& Heenen to be published

Low-lying states in ^{46}Ca





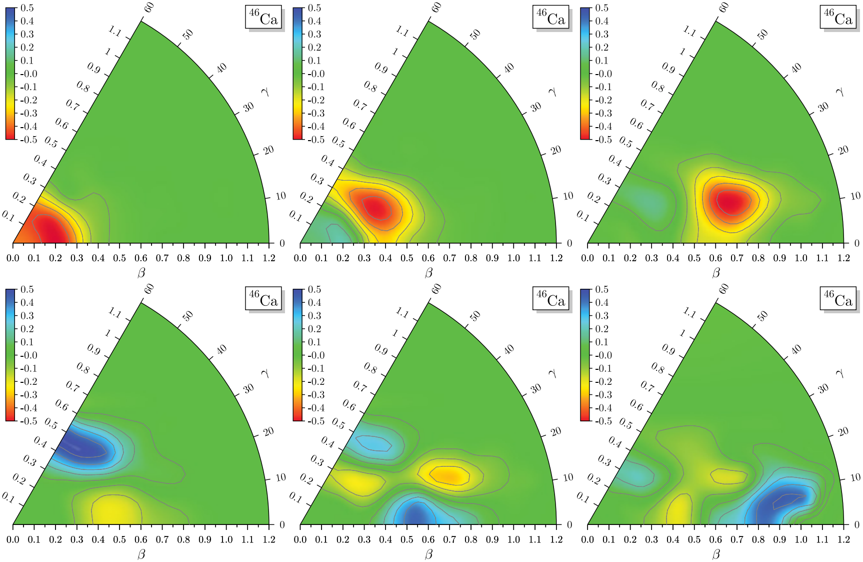
Nilsson diagram along the path indicated by cyan dots. Vertical bars indicate the deformation of the minima.



Nilsson diagram for a closed path through indicated by yellow dots.

Bender& Heenen to be published

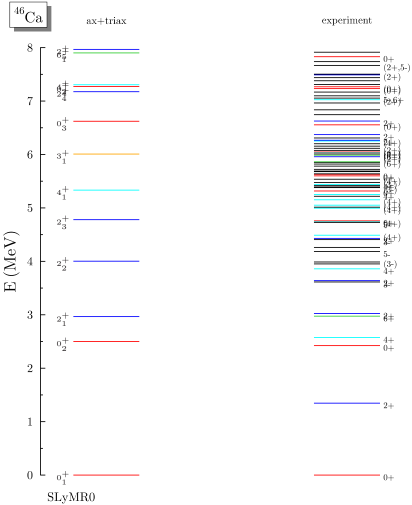
Low-lying states in ^{46}Ca



Lowest eigenstates of the Hamiltonian for $J = 0$.

Bender& Heenen to be published

Low-lying states in ^{46}Ca



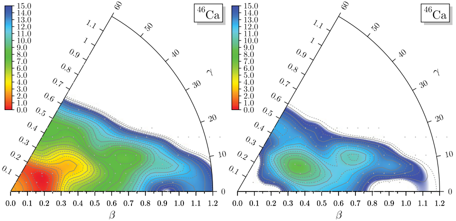
Bender& Heenen to be published

- There is a sequence of "seniority-2" states with $J^\pi = 2^+, 4^+, 6^+$ that in the shell-model is easily obtained by coupling two neutron holes in the $1f_{7/2}-$shell to these angular momenta.
- These are non-collective; hence, cannot be described by "traditional" GCM.

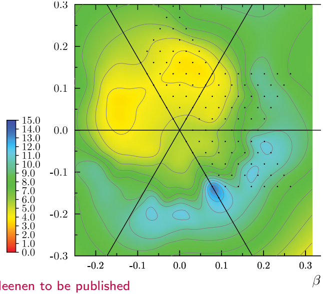
Low-lying states in ^{46}Ca

seniority 0

N, Z, $J = 0$ projected N, Z, $J = 6$ projected



seniority 2, lowest N, Z, $J = 6$ projected

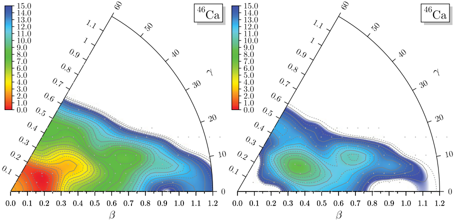


Bender& Heenen to be published

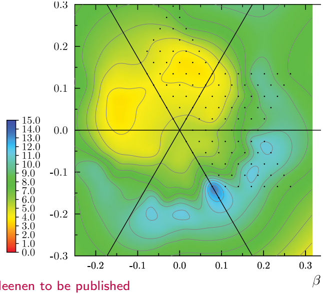
Low-lying states in ^{46}Ca

seniority 0

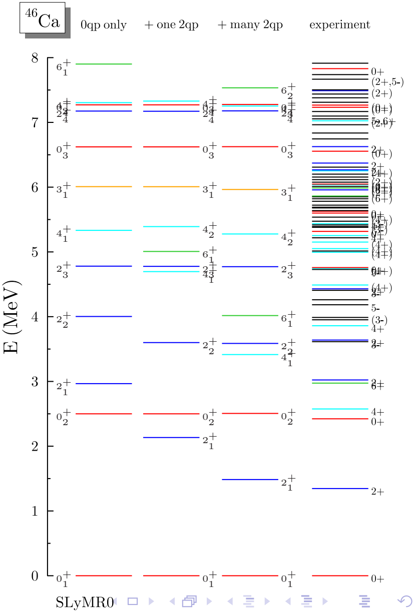
N, Z, $J = 0$ projected N, Z, $J = 6$ projected

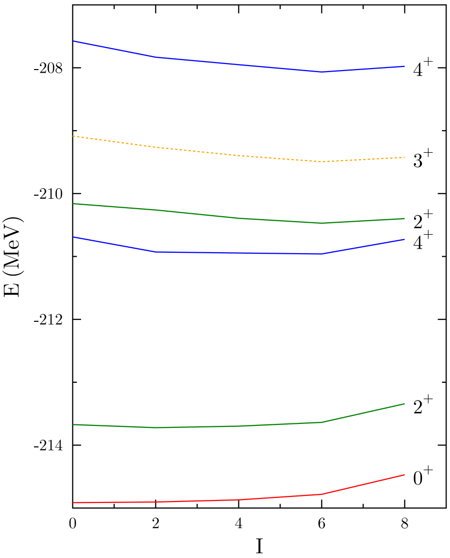


seniority 2, lowest N, Z, $J = 6$ projected



Bender& Heenen to be published





- states cranked to $I = \sqrt{J(J+1)}$
- (triaxial) deformation held fixed to the one giving the lowest projected 0^+ state
- spectrum becomes compressed
- energy gain depends on amount of pairing correlations present at $I = 0$ (which are quite weak for the state used as example)

Avez, Bally, Bender& Heenen, to be published

Ongoing improvements: 3-body terms of 2nd order in gradients

- the most general central Skyrme-type 3-body force up to 2nd order in gradients has been constructed by J. Sadoudi

$$
\begin{aligned}
\hat{v}_{123} = {} & u_0 \left(\hat{\delta}_{r_1 r_3}\hat{\delta}_{r_2 r_3} + \hat{\delta}_{r_3 r_2}\hat{\delta}_{r_1 r_2} + \hat{\delta}_{r_2 r_1}\hat{\delta}_{r_3 r_1}\right) \\
& + \frac{u_1}{2}\left[1 + y_1 P^{\sigma}_{12}\right]\left(\hat{\mathbf{k}}_{12}\cdot\hat{\mathbf{k}}_{12} + \hat{\mathbf{k}}'_{12}\cdot\hat{\mathbf{k}}'_{12}\right)\hat{\delta}_{r_1 r_3}\hat{\delta}_{r_2 r_3} \\
& + \frac{u_1}{2}\left[1 + y_1 P^{\sigma}_{31}\right]\left(\hat{\mathbf{k}}_{31}\cdot\hat{\mathbf{k}}_{31} + \hat{\mathbf{k}}'_{31}\cdot\hat{\mathbf{k}}'_{31}\right)\hat{\delta}_{r_3 r_2}\hat{\delta}_{r_1 r_2} \\
& + \frac{u_1}{2}\left[1 + y_1 P^{\sigma}_{23}\right]\left(\hat{\mathbf{k}}_{23}\cdot\hat{\mathbf{k}}_{23} + \hat{\mathbf{k}}'_{23}\cdot\hat{\mathbf{k}}'_{23}\right)\hat{\delta}_{r_2 r_1}\hat{\delta}_{r_3 r_1} \\
& + u_2\left[1 + y_{21} P^{\sigma}_{12} + y_{22}(P^{\sigma}_{13} + P^{\sigma}_{23})\right]\left(\hat{\mathbf{k}}_{12}\cdot\hat{\mathbf{k}}'_{12}\right)\hat{\delta}_{r_1 r_3}\hat{\delta}_{r_2 r_3} \\
& + u_2\left[1 + y_{21} P^{\sigma}_{31} + y_{22}(P^{\sigma}_{32} + P^{\sigma}_{12})\right]\left(\hat{\mathbf{k}}_{31}\cdot\hat{\mathbf{k}}'_{31}\right)\hat{\delta}_{r_3 r_2}\hat{\delta}_{r_1 r_2} \\
& + u_2\left[1 + y_{21} P^{\sigma}_{23} + y_{22}(P^{\sigma}_{21} + P^{\sigma}_{31})\right]\left(\hat{\mathbf{k}}_{23}\cdot\hat{\mathbf{k}}'_{23}\right)\hat{\delta}_{r_2 r_1}\hat{\delta}_{r_3 r_1}
\end{aligned}
$$

Sadoudi, Duguet, Meyer, Bender, PRC 88 (2013) 064326

Jodon, Doctoral thesis, Lyon (2014)

- parameter fits and exploratory calculations are underway.

Take-away messages

Many efforts are underway to improve the description of excited states in mean-field-based models

- construction of more general (less symmetry restricted) configurations
- improved parameterizations (better fits)
- improved effective interactions (additional and/or different terms)

Calculations based on the mixing of angular-momentum and particle-number restored time-reversal-breaking HFB states gives access to

- coupling of collective and single-particle degrees of freedom
- angular-momentum optimization
- restoration of selection rules for transitions
- beyond-mean-field description of odd-A (and odd-odd) nuclei

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on code development

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Paul-Henri Heenen	Université Libre de Bruxelles
Wouter Ryssens	formerly Université Libre de Bruxelles, now IPN Lyon

on formal aspects (regularization, . . .)

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Denis Lacroix	IPN Orsay
Thomas Lesinski	IPN Lyon

on development, implementation and benchmarking of EDFs

Karim Bennaceur	IPN Lyon
Dany Davesne	IPN Lyon
Veerle Hellemans	Université Libre de Bruxelles
Jacques Meyer	IPN Lyon
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Kouhei Washiyama	Université Libre de Bruxelles