Coupling of collective and single-particle degrees of freedom in symmetry-restored GCM

Michael Bender

Institut de Physique Nucléaire de Lyon, CNRS/IN2P3, Université de Lyon, Université Lyon 1
69622 Villeurbanne, France

incomplete work in progress begun while having been at the

Centre d'Etudes Nucléaires de Bordeaux Gradignan, CNRS/IN2P3, Université de Bordeaux
33175 Gradignan, France

Workshop on
Pertinent ingredients for Multi-Reference EDF calculations
ESNT Saclay, 28 February 2017

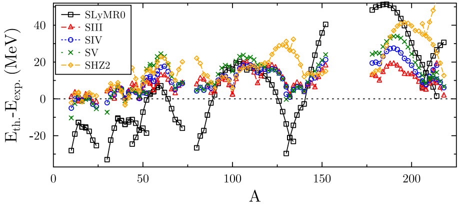
Pseudo-potentials for MR EDF. First try: SLyMR0

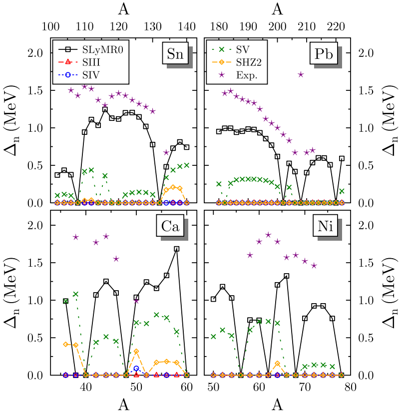
Effective interaction used throughout this talk: SLyMR0

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

J. Sadoudi, M. Bender, K. Bennaceur, D. Davesne, R. Jodon, and T. Duguet, Physica Scripta T154 (2013) 014013

Pseudo-potentials for MR EDF. First try: SLyMR0

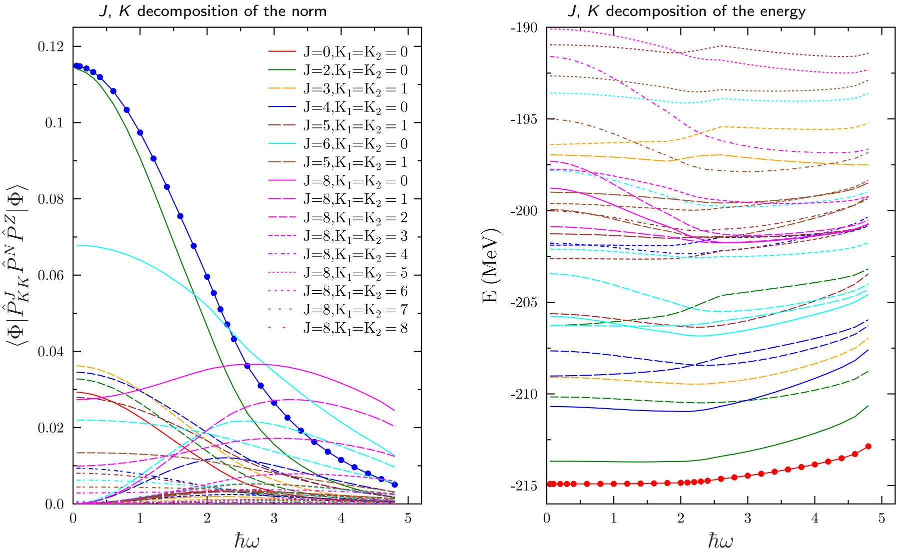




- it is impossible to fullfil the usual nuclear matter constraints , to have stable interactions and attractive pairing
- no "best fit" possible
- very bad performance compared to standard general functionals

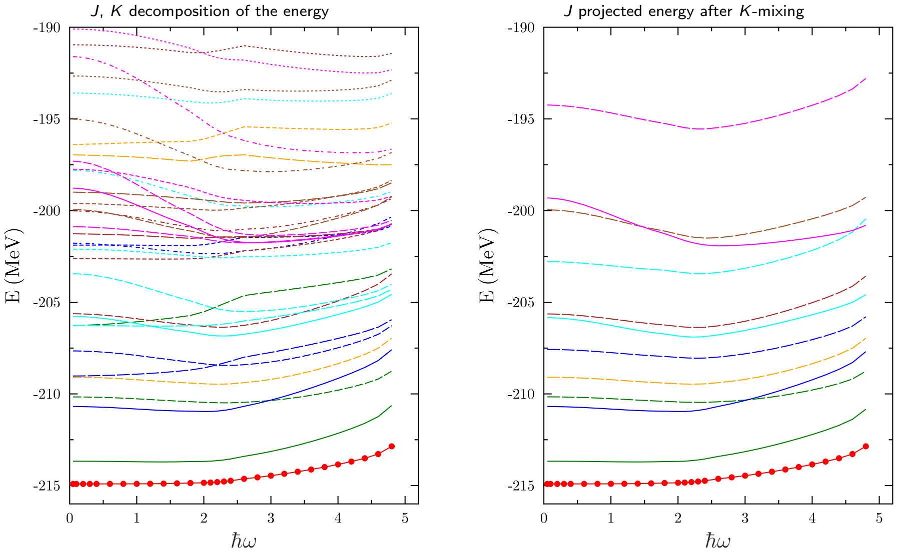
J. Sadoudi, M. Bender, K. Bennaceur, D. Davesne, R. Jodon, and T. Duguet, Physica Scripta T154 (2013) 014013

Rotational band in ^{24}Mg



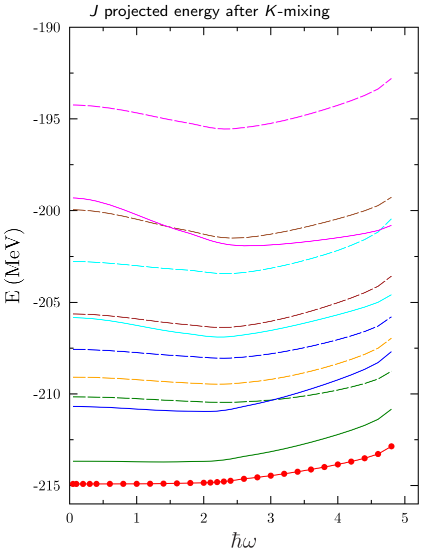
Bender, Avez, Bally, Heenen, to be published

Rotational band in ^{24}Mg

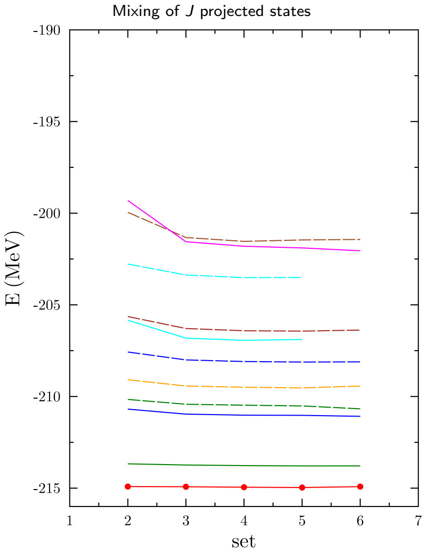


Bender, Avez, Bally, Heenen, to be published

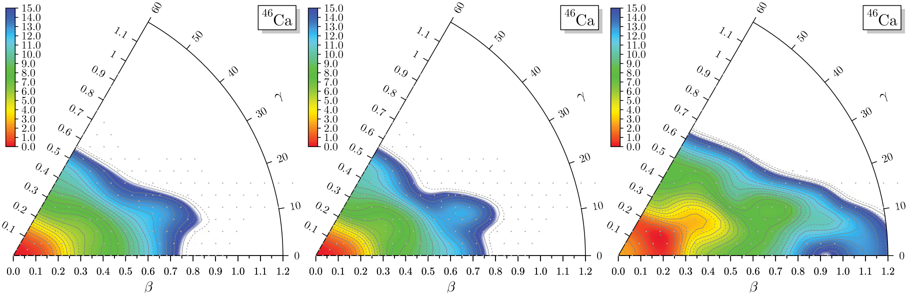
Rotational band in ^{24}Mg



Bender, Avez, Bally, Heenen, to be published

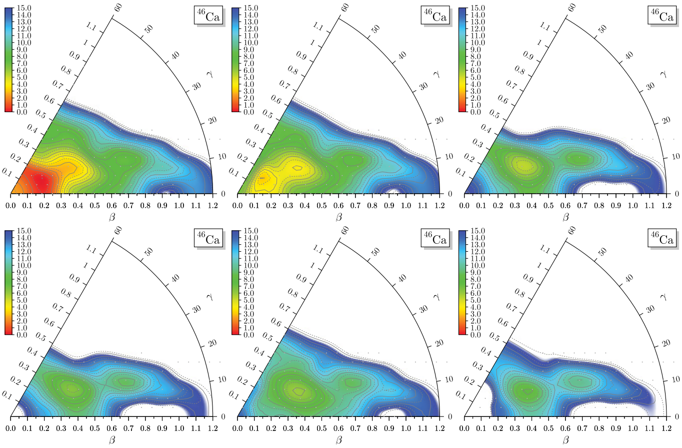


Low-lying states in ^{46}Ca



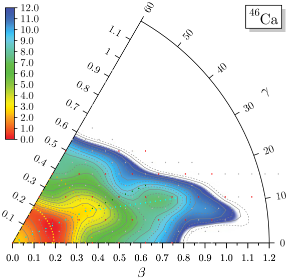
Left: Non-projected total energy of the HFB vacua (without LN correction) relative to the spherical configuration. Middle: $N = 26$, $Z = 20$ projected total energy of the HFB vacua relative to the spherical configuration. Right: Energy of the projected $N = 26$, $Z = 20$, $J = 0$ HFB vacua.

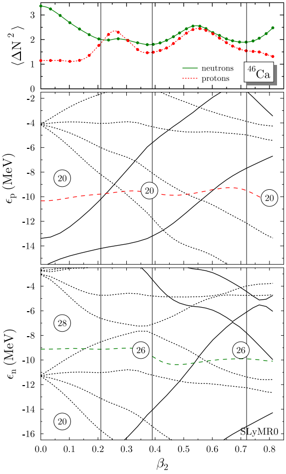
Bender & Heenen, to be published



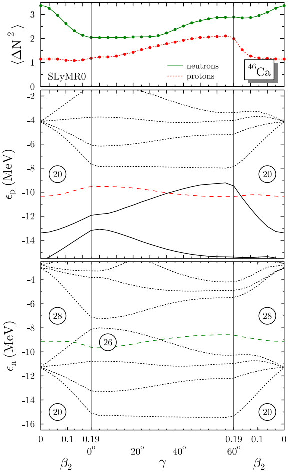
Top row: Right: Energy of the $J = 0$ HFB vacua. Middle: Energy of the lowest K-mixed $J = 2$ projected state . Right: Energy of the second K-mixed $J = 2$ state . Bottom row: Right: Energy of the $J = 3$ state. Middle: Energy of the lowest K-mixed $J = 4$ projected state. Right: Energy of the second 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





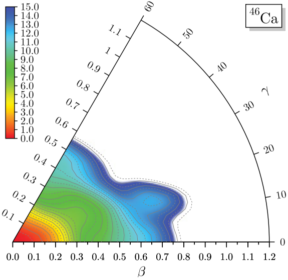
Nilsson diagram along the path indicated by cyan dots. Vertical bars indicate the deformation of the minima.

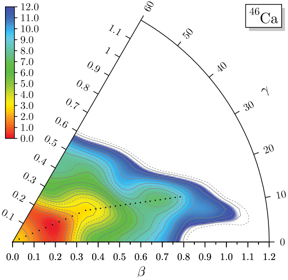


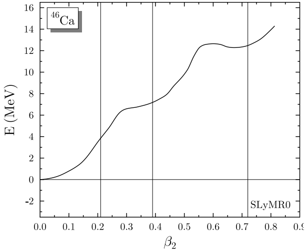
Nilsson diagram for a closed path through indicated by yellow dots.

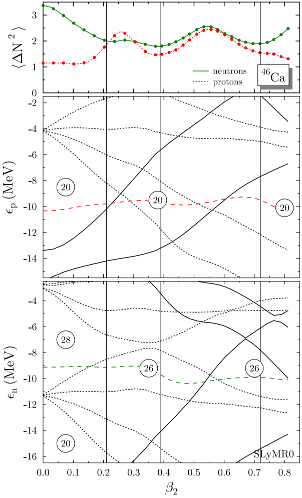
Bender & Heenen to be published

Low-lying states in ^{46}Ca



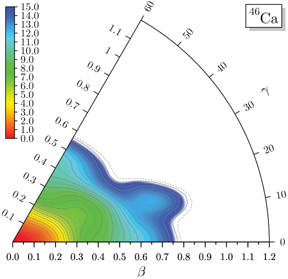


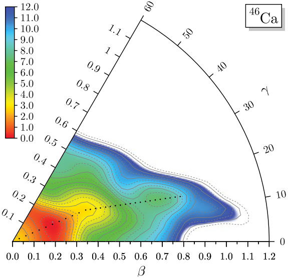


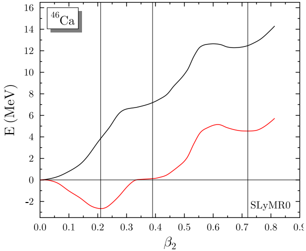


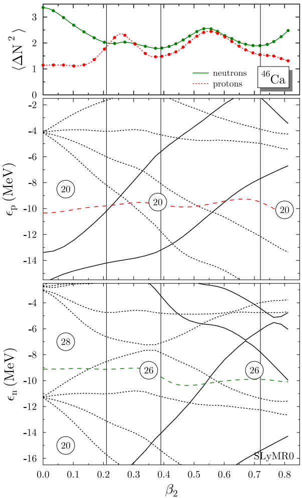
Bender, Bally, Heenen, to be published

Low-lying states in ^{46}Ca



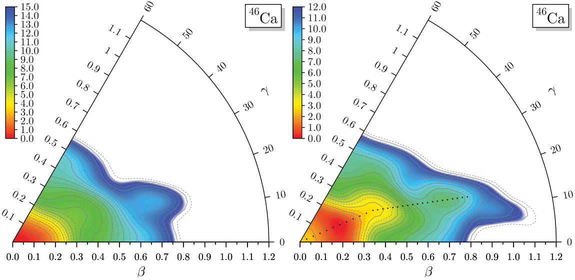


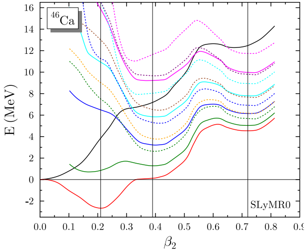


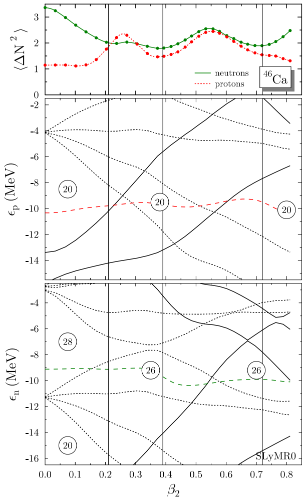


Bender, Bally, Heenen, to be published

Low-lying states in ^{46}Ca



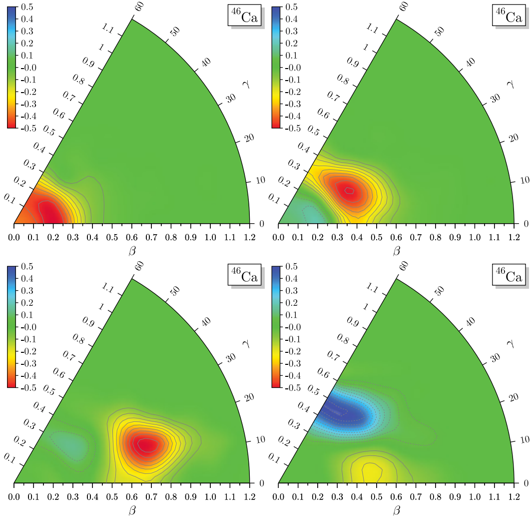


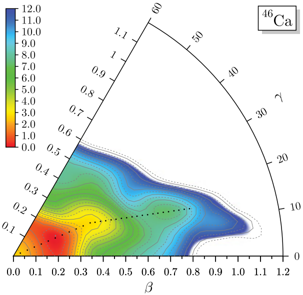


Bender, Bally, Heenen, to be published

Low-lying states in ^{46}Ca

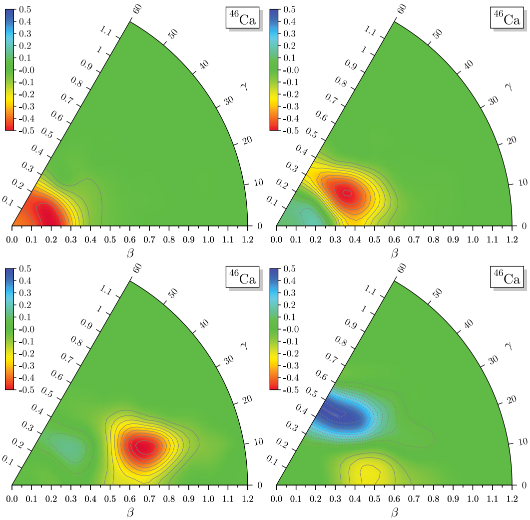
collective wave function of the four lowest 0^+ states

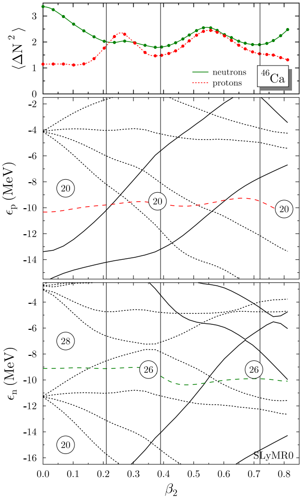




Bender, Bally, Heenen, to be published

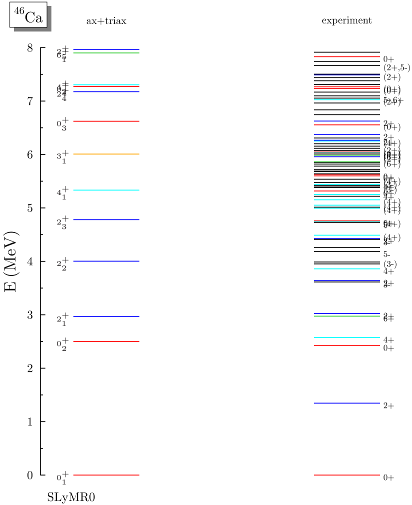
collective wave function of the four lowest 0^+ states





Bender, Bally, Heenen, to be published

Low-lying states in ^{46}Ca



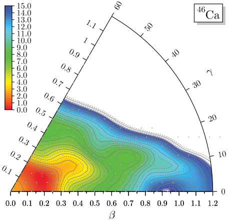
Bender & Heenen, to be published

- 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.

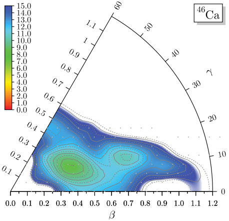
Low-lying states in ^{46}Ca

seniority 0

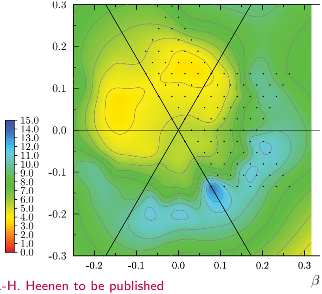
N, Z, J = 0 projected



N, Z, J = 6 projected



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

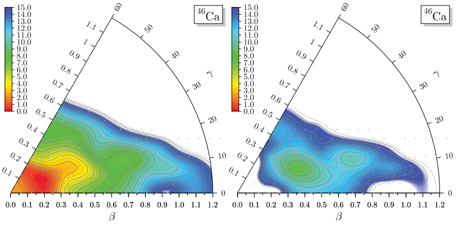


Bender& P.-H. Heenen to be published

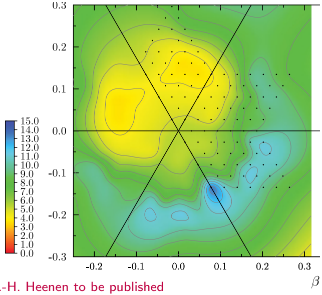
seniority 0

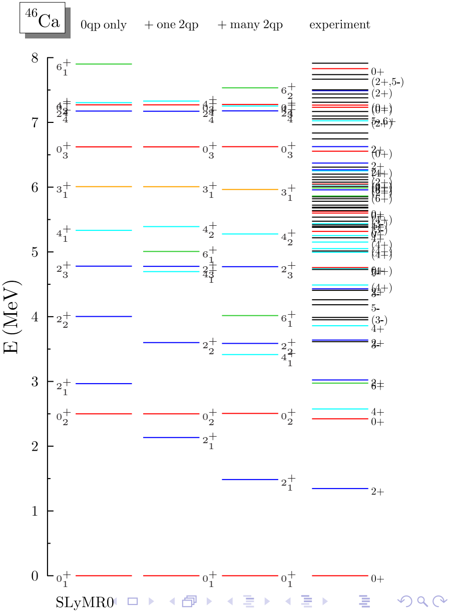
N, Z, $J = 0$ projected

N, Z, $J = 6$ projected



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

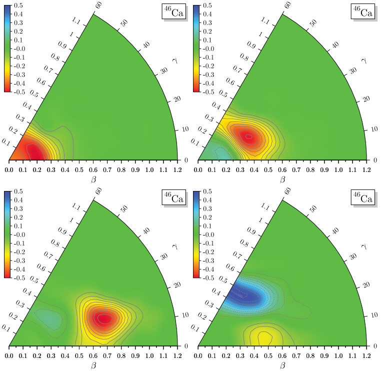


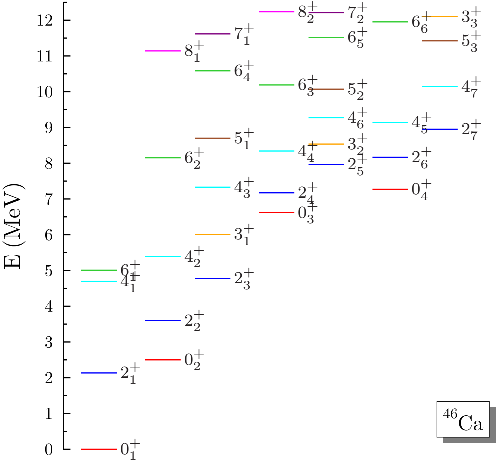


Bender& P.-H. Heenen to be published

Low-lying states in ^{46}Ca

collective wave function of the four lowest 0^+ states





Bender, Bally, Heenen, to be published

Construction of new forms of effective interactions

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

  (not aiming at true Hamiltonians so far, though)

  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 explicit three-body interactions

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

  Sadoudi, Bender, Bennaceur, Davesne, Jodon, Duguet, Phys Scr T154 (2013) 014013

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

- regularised contact interactions (replacing the delta function in SKyrme with Gaussians)

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

  Bennaceur, Idini, J. Dobaczewski, P. Dobaczewski, Kortelainen, Raimondi, JPG44 (2017) 045106

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

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

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

Takeaway messages

- **degrees of freedom considered and level of modeling at which they enter:** quadrupole and other deformations (SR & MR), pairing correlations (SR & MR), intrinsic angular momentum (SR & MR), quasi-particle excitations (SR & MR).

  Breaking of time-reversal invariance in the SR states as prerequisite of coupling single-particle degrees of freedom to collective motion.
- **phenomena these can be expected to be (particularly) relevant for:** Low-lying nuclear structure.
- **their treatment as discussed can be (easily) combined with the one of other degrees of freedom?** Formally: yes (higher-order deformations, higher-order quasiparticle excitations). Computationally: not necessarily.
- **can they be expected to be independent/orthogonal to other degrees of freedom discussed during the workshop:** Not necessarily.

Acknowledgements

The work presented here would have been impossible without my collaborators

founding fathers

Paul Bonche	SPhT, CEA Saclay
Hubert Flocard	CSNSM Orsay
Paul-Henri Heenen	Université Libre de Bruxelles

formal aspects of the big picture

Thomas Duguet	Irfu/CEA Saclay & KU Leuven & NSCL/MSU
Denis Lacroix	IPN Orsay

design and implementation of code extensions

Benoît Avez	CEN Bordeaux Gradignan
Benjamin Bally	CEN Bordeaux Gradignan, now SPhN, CEA Saclay
Veerle Hellemans	Université Libre de Bruxelles
Wouter Ryssens	IPN Lyon

development and benchmarking of new functionals

Karim Bennaceur	IPN Lyon & Jyväskylä
Dany Davesne	IPN Lyon
Robin Jodon	IPN Lyon
Jacques Meyer	IPN Lyon
Alessandro Pastore	formerly IPN Lyon, now University of York
Jeremy Sadoudi	Irfu/CEA Saclay first, then CEN Bordeaux Gradignan
Kouhei Washiyama	Université Libre de Bruxelles

color code: active (past) member of the collaboration