# Mean-field-based tools for the description of excited states of heavy nuclei

Michael Bender

Université Bordeaux 1; CNRS/IN2P3; Centre d'Etudes Nucléaires de Bordeaux Gradignan, UMR5797
Chemin du Solarium, BP120, 33175 Gradignan, France

Workshop on

*Advances in experimental and theoretical studies of heavy, very heavy and super-heavy nuclei*

Espace de Structure et de réactions Nucléaires Théorique
Saclay, 16-19 November 2015

# Today's standards

Effective interactions

- Gogny: finite-range Gaussian central force + contact density dependence + contact spin-orbit interaction
- Skyrme: contact central interaction with gradients + contact density dependence + contact spin-orbit interaction
- Relativistic mean field (aka covariant DFT):
  - relativistic Hartree models with "finite-range mesons"
  - relativistic point-coupling Hartree models
  - relativistic Hartree-Fock models with "finite-range mesons"

# Mean-field-based models - Ongoing research

Construction of better effective interactions

- construction of better parameterizations of existing forms
- construction of new forms of the nuclear EDF
- recognition of formal constraints on the form of the nuclear EDF

Better modeling of the nuclear "wave function"

- towards symmetry-unrestricted mean-field calculations
- explicit treatment of correlation effects

# Description of excited states

- single-particle excitations $\Rightarrow$ blocked HFB
- rotational bands $\Rightarrow$ cranked HFB
- small-amplitude shape vibrations $\Rightarrow$ Random Phase Approximation (RPA)
- large-amplitude shape vibrations $\Rightarrow$ Generator Coordinate Method (GCM)
- shape coexistence $\Rightarrow$ Generator Coordinate Method

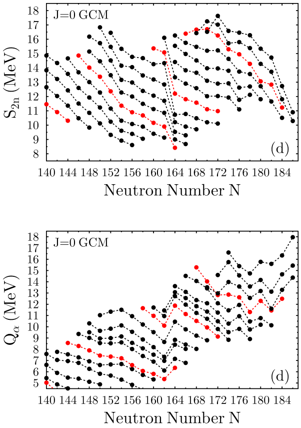
# Symmetry considerations

- quasiparticle excitations (and odd- and odd-odd nuclei in general) $\Leftrightarrow$ broken time-reversal symmetry
- rotating nuclei ("cranking") $\Leftrightarrow$ broken time-reversal symmetry
- collectively rotating nuclei ("cranking") $\Leftrightarrow$ broken axial symmetry
- octupole correlations $\Leftrightarrow$ broken parity
- rotating quasiparticle excitations $\Leftrightarrow$ broken signature symmetry

Up to now, very few calculations combine broken time-reversal symmetry and broken parity, or broken signature in addition to broken time-reversal symmetry.

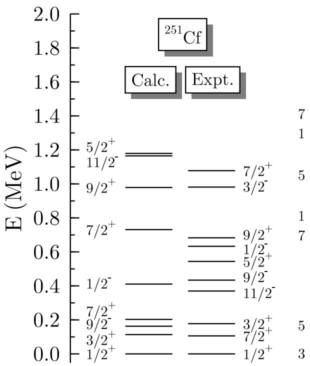
# Indicators of (deformed) shell structure

## Mass differences



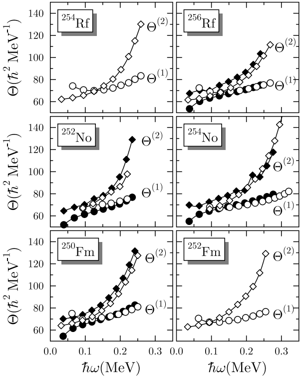

M. B. and Heenen, to be published

## Spectra of bandheads in odd-mass nuclei




M. B., Bonche, Duguet, Heenen, NPA723 (2003) 354

## Moment of inertia




M. B. and Heenen, J. Phys. Conf. Ser. 420 (2013) 012002

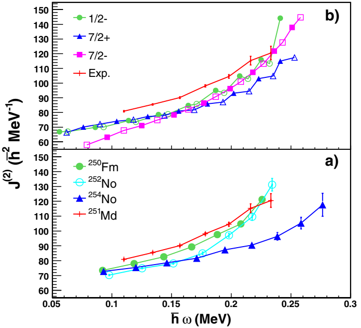



FIG. 3 (color online). (a) Dynamical moment of inertia of the observed rotational band compared to the experimental results obtained in neighboring even-even nuclei. (b) Comparison with the theoretical dynamical moment of inertia, where empty (solid) symbols correspond to a negative (positive) signature.

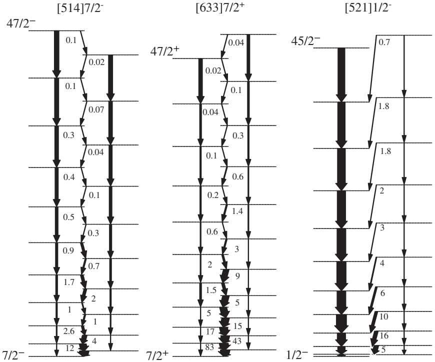
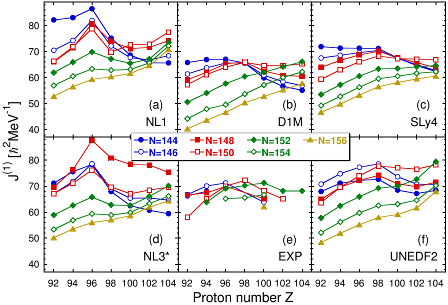


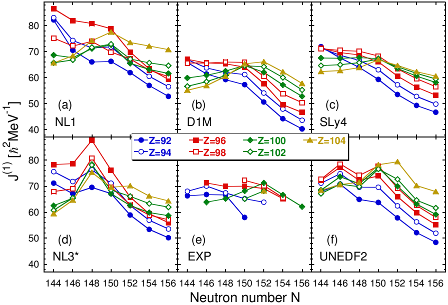

FIG. 4. Schematic decay pattern for the three configuration candidates. The number labeling the state corresponds to the ratio $T(M1)/T(E2)$.

(transition rates estimated using Bohr-Mottelson-type approximation)

Chatillon, Theisen, . . . , Clément, . . . , Bonche, Heenen, PRL 98 (2007) 132503

# Kinematical moment of inertia



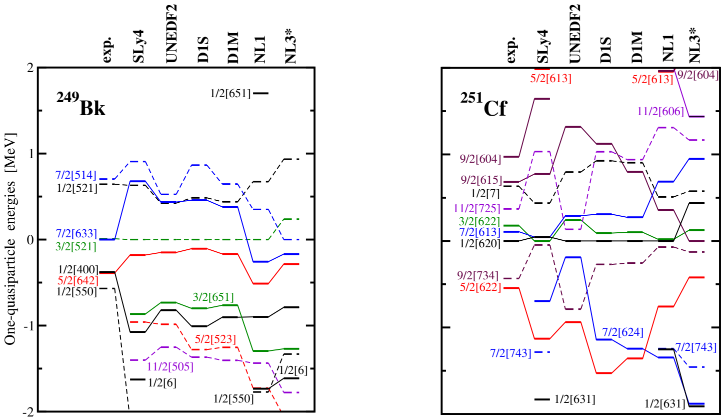




$$J^{(1)} \equiv \frac{\langle \hat{J}_\perp \rangle}{\omega_\perp},$$

evaluated at $\hbar\omega_\perp = 20\,\text{keV}$.

Dobaczewski, Afanasjev, M. B., Robledo, Shi, arXiv:1504.03245

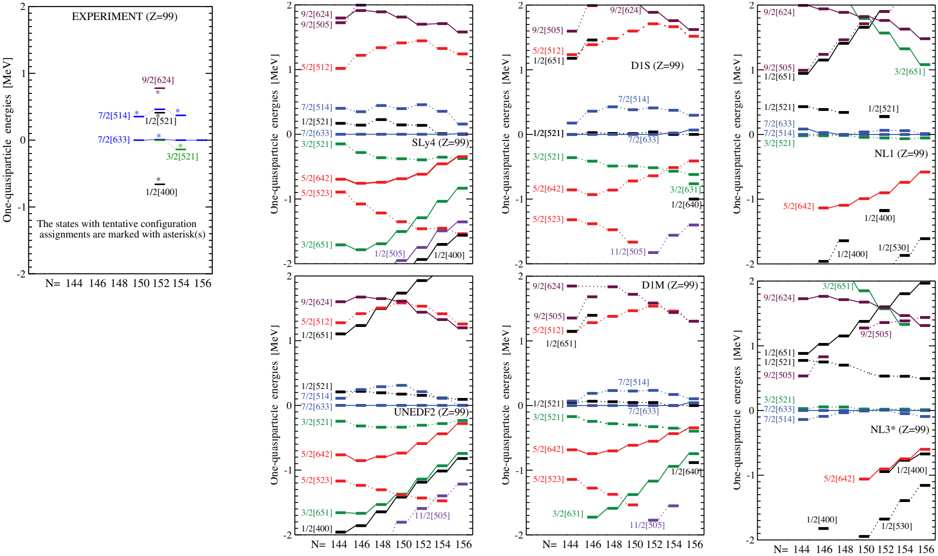
# One-quasiparticle states (bandheads) in $^{249}$Bk and $^{251}$Cf



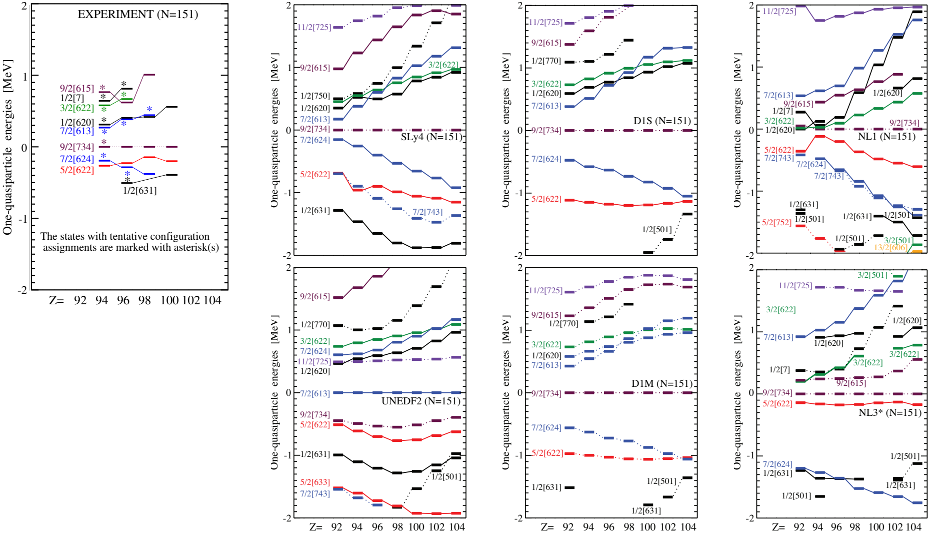

- intruder levels ($\nu$ 11/2[725] and $\pi$ 7/2[633]) misplaced in the spectrum (which can be partially cured with local readjustment of the spin-orbit interaction, [Shi, Dobaczewski, Greenlees, PRC 89 (2014) 034309]), but that's not the only problem.

Dobaczewski, Afanasjev, M. B., Robledo, Shi, arXiv:1504.03245

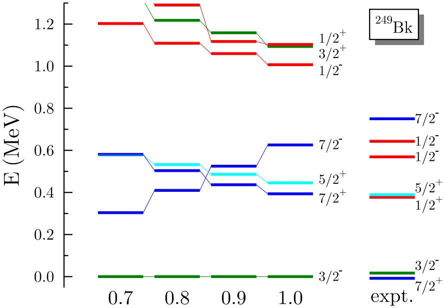
Dobaczewski, Afanasjev, M. B., Robledo, Shi, arXiv:1504.03245

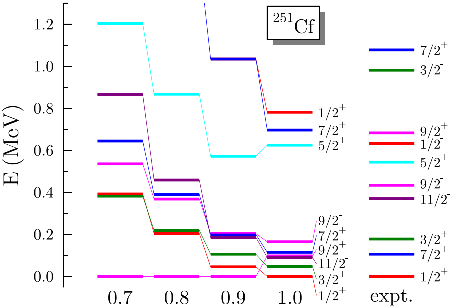


Dobaczewski, Afanasjev, M. B., Robledo, Shi, arXiv:1504.03245



# Scaling with effective mass?

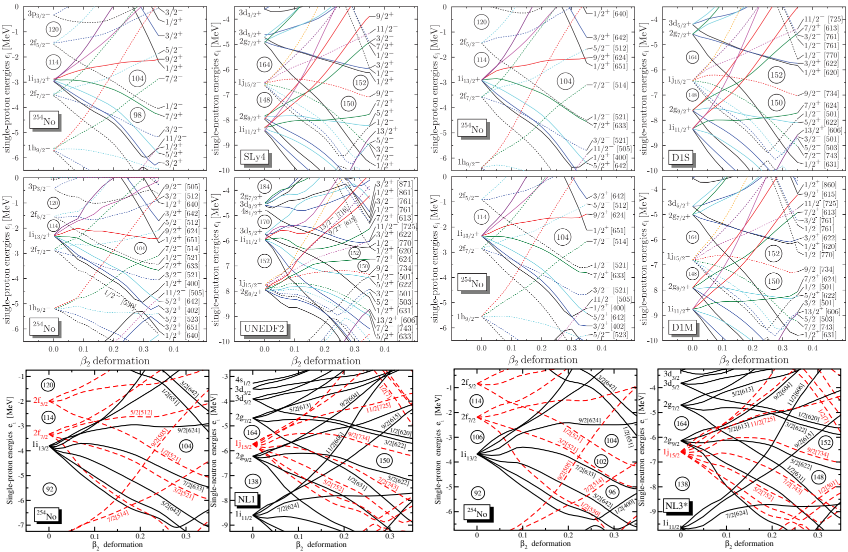



Washiyama, Bennaceur, Avez, M. B., Heenen, Hellemans, PRC 86 (2012) 054309

# Nilsson diagrams of $^{254}$No obtained with Skyrme, Gogny, RMF

| | protons | neutrons | protons | neutrons | |
|---|---|---|---|---|---|
| SLy4 | | | | | D1S |
| UN-EDF2 | | | | | D1M |
| NL1 | | | | | NL3* |

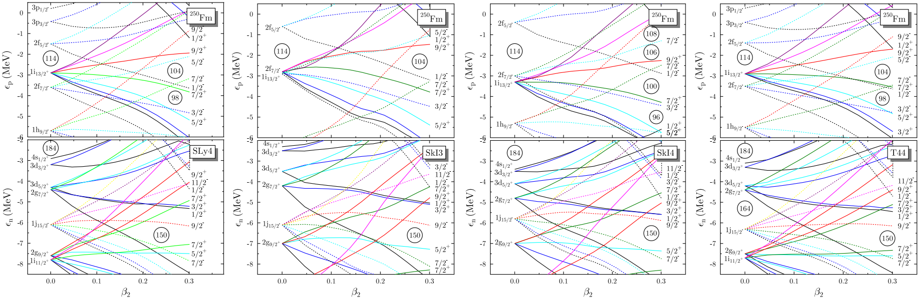



Dobaczewski, Afanasjev, M. B., Robledo, Shi, arXiv:1504.03245

# Parameterization sensitivity: the example of $^{250}$Fm

M. B., Heenen, J. Phys. Conf. Ser. 420 (2013) 012002

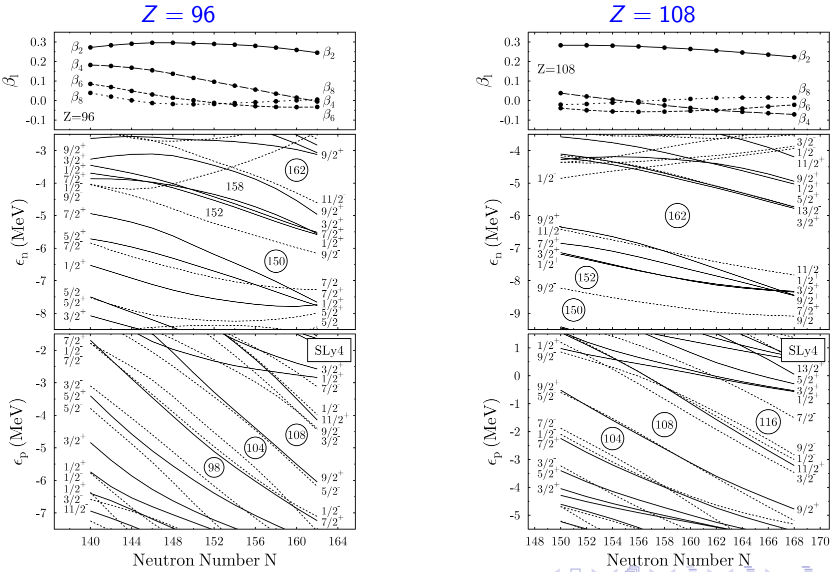
| SLy4 | SkI3 | SkI4 | T44 |
|---|---|---|---|
| standard spin-orbit | modified spin-orbit | modified spin-orbit | tensor force added |




- Nilsson diagram of protons (top) and neutrons (bottom) going from spherical shape (left) to the prolate deformed ground state (right)
- different colours indicate different mean values of $j_z$
- compare bunching of levels, not the details.

# Evolution of deformed shells with SLy4

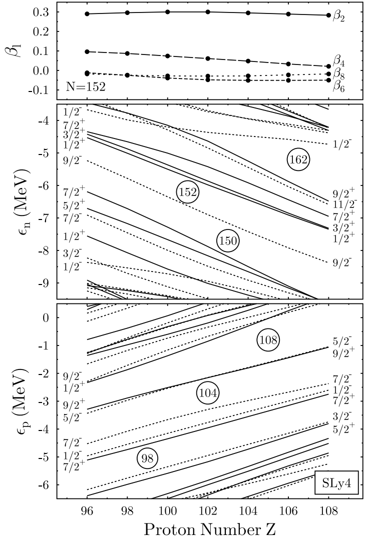
M. B. and Heenen, to be published



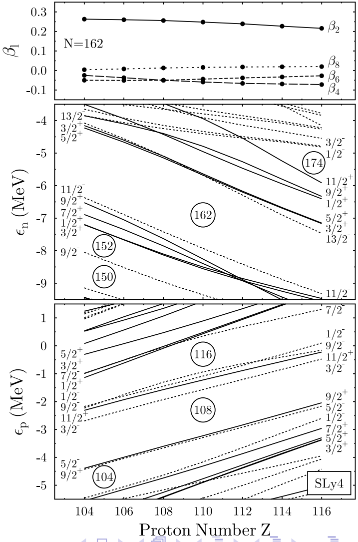
# Evolution of deformed shells with SLy4

M. B. and Heenen, to be published

$N = 152$



$N = 162$



# Construction of better parameterizations

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

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

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

  Lesinski, M. B., Bennaceur, Duguet, Meyer, PRC 76 (2007) 014312

  M. B., 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, M. B., in preparation.

- 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

  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 explicit three-body interactions

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

  Sadoudi, M. B., Bennaceur, Davesne, Jodon, Duguet, Phys Scr T154 (2013) 014013

  Sadoudi, Duguet, Meyer, M. B., PRC 88 (2013) 064326

- finite-range density dependences

  Chappert, thèse, Université de Paris-Sud XI (2007)

  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)

# 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 explicit three-body interactions

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

  Sadoudi, M. B., Bennaceur, Davesne, Jodon, Duguet, Phys Scr T154 (2013) 014013

  Sadoudi, Duguet, Meyer, M. B., PRC 88 (2013) 064326
- finite-range density dependences

  Chappert, thèse, Université de Paris-Sud XI (2007)

  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, M. B., Ebran, Lesinski, Somà, arXiv:1502.03672 particle-number projector

$$\hat{P}_{N_0} = \frac{1}{2\pi} \int_0^{2\pi} d\phi_N \underbrace{e^{-i\phi_N N_0}}_{\text{weight}} \overbrace{e^{i\phi_N \hat{N}}}^{\text{rotation in gauge space}}$$

angular-momentum restoration operator

$$\hat{P}^J_{MK} = \frac{2J+1}{16\pi^2} \int_0^{4\pi} d\alpha \int_0^{\pi} d\beta \, \sin(\beta) \int_0^{2\pi} d\gamma \underbrace{\mathcal{D}^{*J}_{MK}(\alpha,\beta,\gamma)}_{\text{Wigner function}} \overbrace{\hat{R}(\alpha,\beta,\gamma)}^{\text{rotation in real space}}$$

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

$$|JMq\rangle = \sum_{K=-J}^{+J} f_J(K) \, \hat{P}^J_{MK} \, \hat{P}^Z \, \hat{P}^N \, |\mathrm{MF}(q)\rangle = \sum_{K=-J}^{+J} f_J(K) \, |JM(qK)\rangle$$

$f_J(K)$ 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, $f_J(K) \sim \delta_{K0}$

## Configuration mixing by the symmetry-restored Generator Coordinate Method

Superposition of projected self-consistent mean-field states $|\mathrm{MF}(\mathbf{q})\rangle$ differing in a set of collective and single-particle coordinates $\mathbf{q}$

$$|NZJM\nu\rangle = \sum_{\mathbf{q}} \sum_{K=-J}^{+J} f_{J,\kappa}^{NZ}(\mathbf{q},K)\,\hat{P}^J_{MK}\,\hat{P}^Z\,\hat{P}^N\,|\mathrm{MF}(\mathbf{q})\rangle = \sum_{\mathbf{q}} \sum_{K=-J}^{+J} f_{J\nu}^{NZ}(\mathbf{q},K)\,|NZ\,JM(\mathbf{q}K)\rangle$$

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

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

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

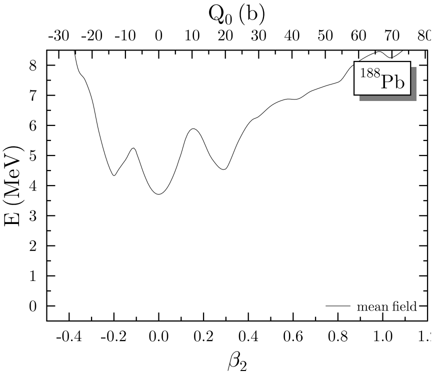
with

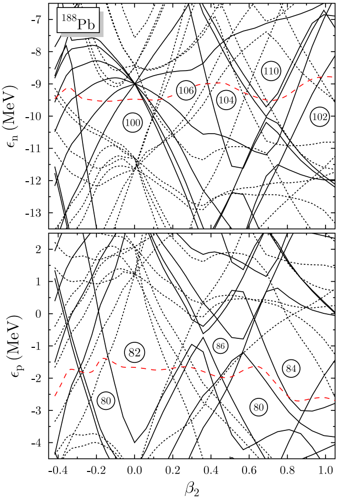
$$\mathcal{H}_J(\mathbf{q}K,\mathbf{q}'K') = \langle NZ\,JM\,\mathbf{q}K|\hat{H}|NZ\,JM\,\mathbf{q}'K'\rangle \qquad \text{energy kernel}$$
$$\mathcal{I}_J(\mathbf{q}K,\mathbf{q}'K') = \langle NZ\,JM\,\mathbf{q}K|NZ\,JM\,\mathbf{q}'K'\rangle \qquad \text{norm kernel}$$

Angular-momentum projected GCM gives the

- correlated ground state for each value of $J$
- spectrum of excited states for each $J$

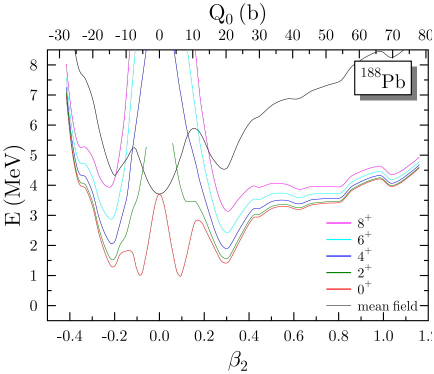
# Configuration mixing via the projected Generator Coordinate Method



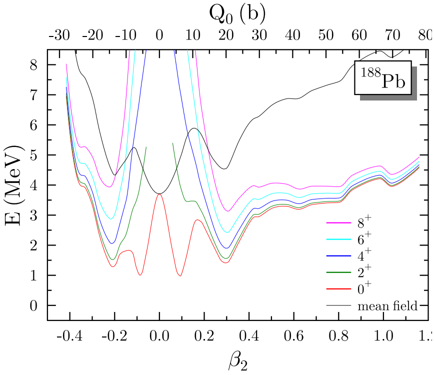



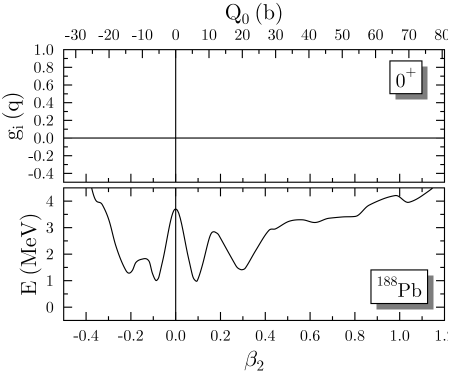

M. B., Bonche, Duguet, Heenen, PRC 69 (2004) 064303

# Spectroscopy from MR EDF



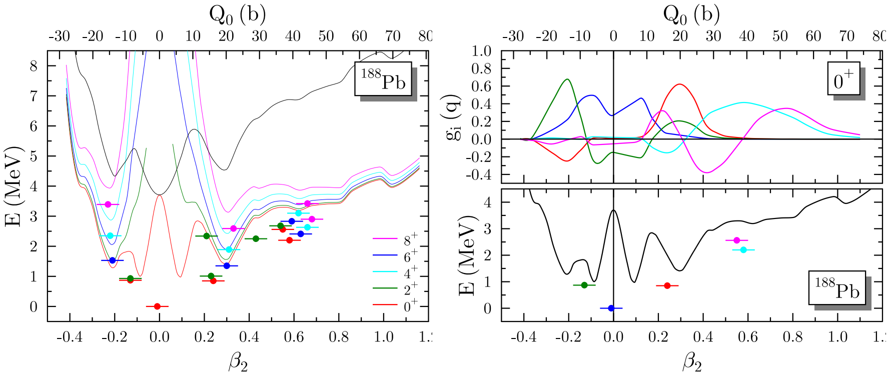

M. B., Bonche, Duguet, Heenen, PRC 69 (2004) 064303




M. B., Bonche, Duguet, Heenen, PRC 69 (2004) 064303

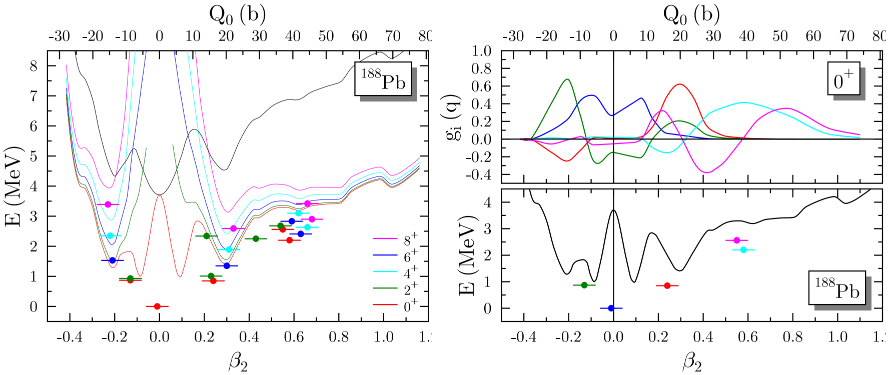
# Spectroscopy from MR EDF




M. B., Bonche, Duguet, Heenen, PRC 69 (2004) 064303

Attention: $g_i^2(q)$ is not the probability to find a mean-field state with intrinsic deformation $q$ in the collective state

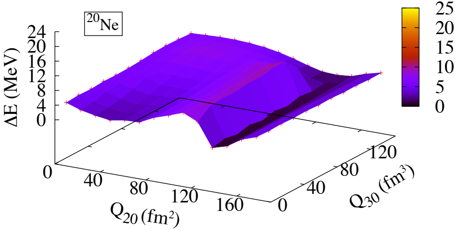
# Spectroscopy from MR EDF

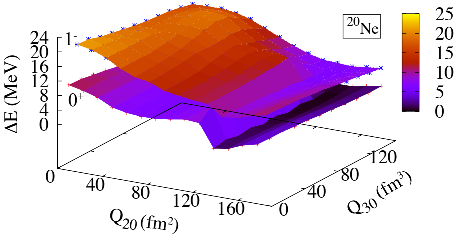



M. B., Bonche, Duguet, Heenen, PRC 69 (2004) 064303

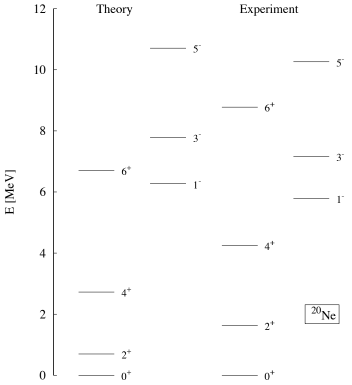
Attention: $g_i^2(q)$ is not the probability to find a mean-field state with intrinsic deformation $q$ in the collective state

# Other collective degrees of freedom: Octupole deformation




V. Hellemans, M. B., P.-H. Heenen, to be published?




- Skyrme SLy5
- axial Slater determinants (no pairing).
- *J* and parity projection

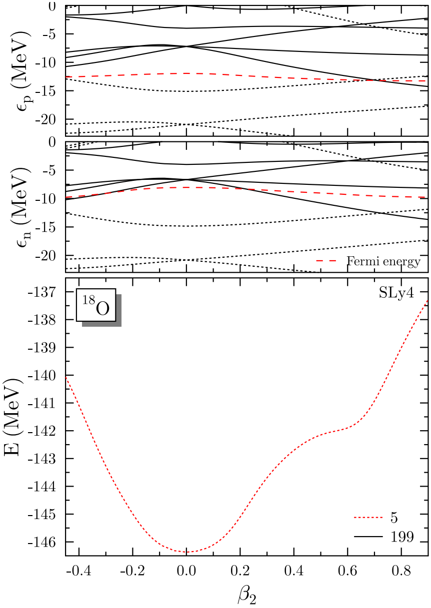
breaking time-reversal invariance of the reference states

- one or several broken pairs: states with seniority $\neq 0$ (and usually $J \neq 0$) in even-even nuclei, $K$-isomers
- one non-paired nucleon: odd-$A$ nuclei
- two non-paired nucleons of different kinds: odd-odd nuclei
- disturbed pairs: angular-momentum optimized collectively rotating states (self-consistent cranking): alignment of single-particle states with the rotation axis and the weakening of pairing with increasing $J$

$$\hat{H} \to \hat{H} - \boldsymbol{\omega} \cdot \hat{\mathbf{J}}$$

$\Rightarrow$ explicit coupling of single-particle states to collective motion

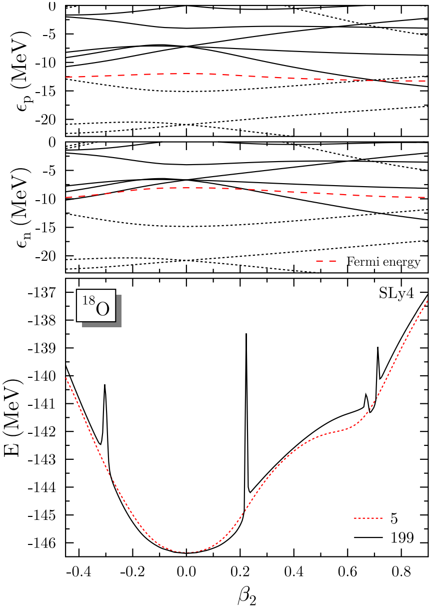
# A word of caution before




- pure particle-number projection

M. B., T. Duguet, and D. Lacroix Phys. Rev. C 79 (2009) 044319

# A word of caution before




- pure particle-number projection
- first hints from Hamiltonian-based approaches in the form of failure of approximations: Dönau, PRC 58 (1998) 872; Almehed, Frauendorf, Dönau, PRC 63 (2001) 044311.
- analysis in density-dependent-Hamiltonian-based approach: Anguiano, Egido, Robledo NPA696 (2001) 467
- First analysis in a strict energy density functional (EDF) framework and of EDF-specific consequences by Dobaczewski, Stoitsov, Nazarewicz, Reinhard, PRC 76 (2007) 054315
- Further analysis of the EDF case by Lacroix, Duguet, M. B., PRC 79 (2009) 044318; M. B., Duguet, Lacroix, PRC 79 (2009) 044319; Duguet, M. B., Bennaceur, Lacroix, Lesinski, PRC 79 (2009) 044320; M. B., Avez, Bally, Duguet, Heenen, Lacroix, *still in preparation*

## The origin of the problem in a nutshell

- 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

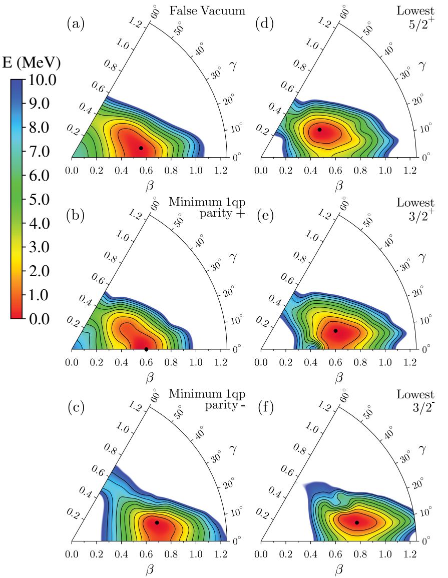
  that are all introduced for phenomenological reasons and/or the sake of numerical efficiency.
- consequence: breaking of the exchange symmetry ("Pauli principle") under particle exchange when calculating the energy, leading to non-physical interactions of a given nucleon or pair of nucleons with itself, or of three nucleons among themselves etc.
- the resulting self-interactions and self-pairing-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-dependences

First try: SLyMR0

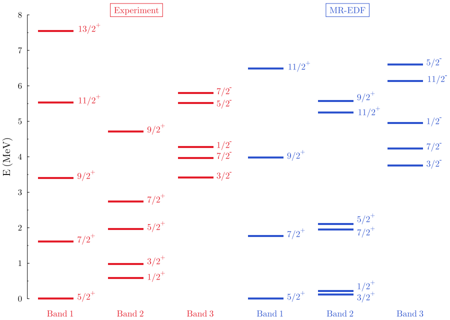
$$
\begin{aligned}
\hat{v} = {} & t_0 \left(1 + x_0 \hat{P}_\sigma\right) \hat{\delta}_{r_1 r_2} \\
& + \frac{t_1}{2} \left(1 + x_1 \hat{P}_\sigma\right) \left(\hat{\mathbf{k}}_{12}^{\prime\,2} \hat{\delta}_{r_1 r_2} + \hat{\delta}_{r_1 r_2} \hat{\mathbf{k}}_{12}^{2}\right) \\
& + t_2 \left(1 + x_2 \hat{P}_\sigma\right)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

Sadoudi, M. B., Bennaceur, Davesne, Jodon, Duguet, Physica Scripta T154 (2013) 014013

# Fun with SLyMR0 – $^{25}$Mg



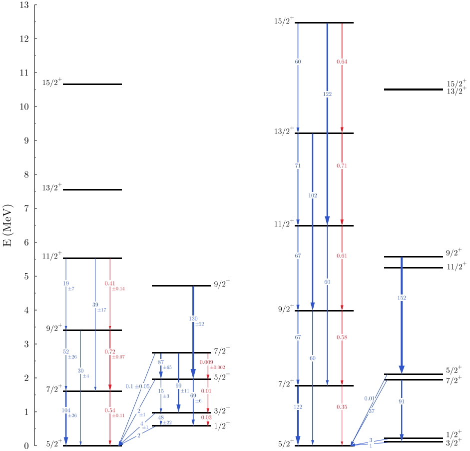

Angular-momentum and particle-number projected GCM of blocked triaxial one-quasiparticle states




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

Bally, Avez, M. B., Heenen, PRL 113 (2014) 162501

# First "beyond-mean-field" results for odd-$A$ nuclei with SLyMR0

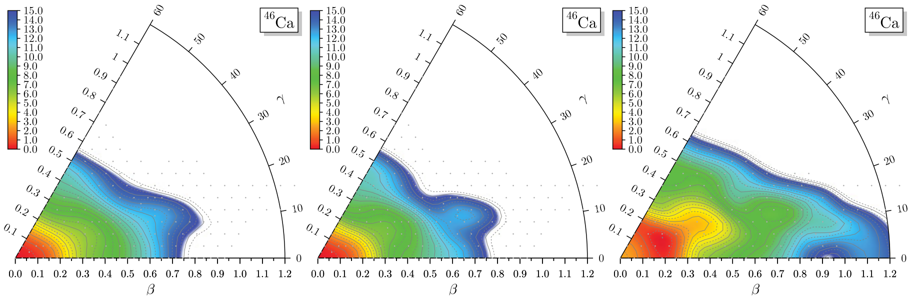



- spectroscopic quadrupole moment $Q_s$ of the $5/2^+$ ground state:
  Exp: $20.1 \pm 0.3$ $e$ fm$^2$
  Calc: $23.25$ $e$ fm$^2$
- magnetic moment $\mu$ of the $5/2^+$ ground state in nuclear magnetons:
  Exp: $-0.855$
  Calc: $-1.054$

Bally, Avez, M. B., Heenen, PRL 113 (2014) 162501

Data from Nuclear Data Sheets 110 (2009) 1691

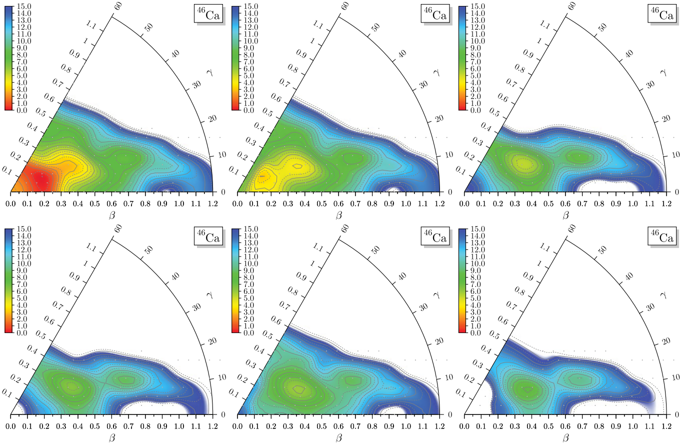
# Fun with SLyMR0 – $^{46}$Ca




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.

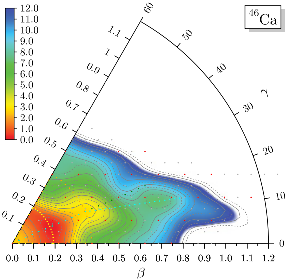
M. B.& P.-H. Heenen to be published

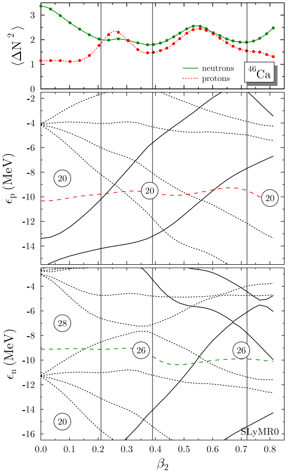
# Fun with SLyMR0 – $^{46}$Ca

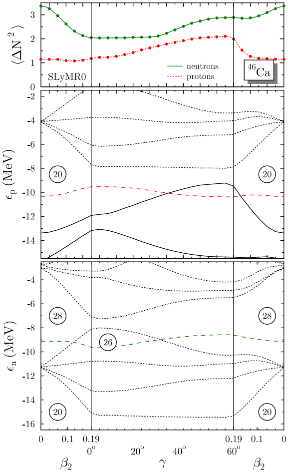



Top row: Right: Energy of the $J = 0$ HFB vacua. Middle: Energy of the lowest $K$-mixed $J = 2$ projected state . Right: Energy of the second $K$-mixed $J = 2$ state . Bottom row: Right: Energy of the $J = 3$ state. Middle: Energy of the lowest $K$-mixed $J = 4$ projected state. Right: Energy of the 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 $N = 26$, $Z = 20$,

M. B.& P.-H. Heenen to be published



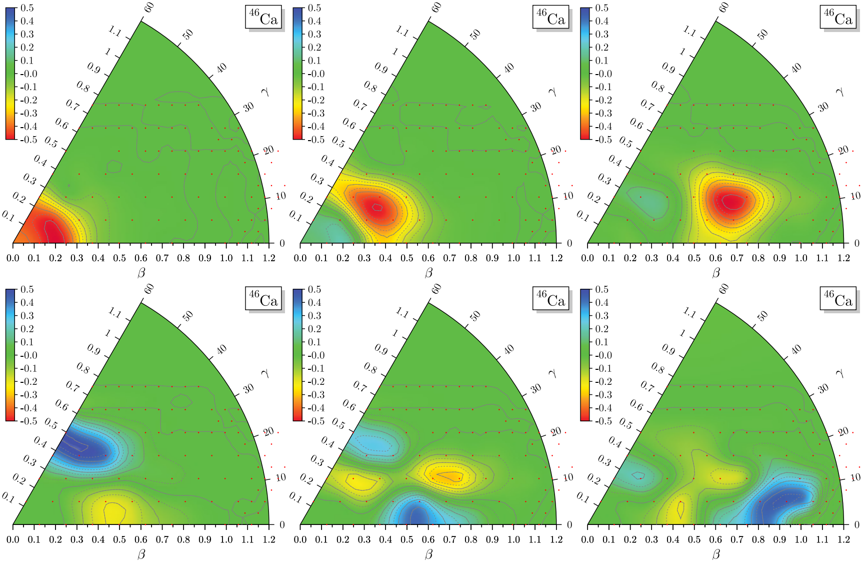




M. B.& P.-H. Heenen to be published

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

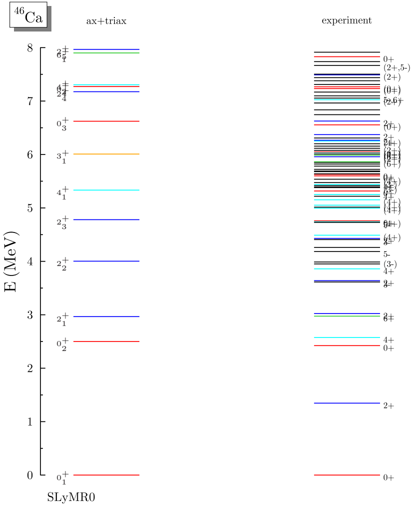
Nilsson diagram for a closed path through indicated by yellow dots.




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

M. B.& P.-H. Heenen to be published

# Fun with SLyMR0 – $^{46}$Ca

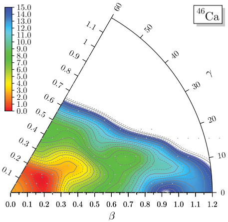


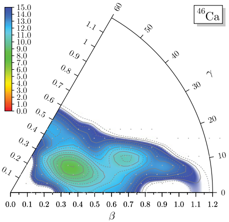

M. B.& P.-H. Heenen to be published

- 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.

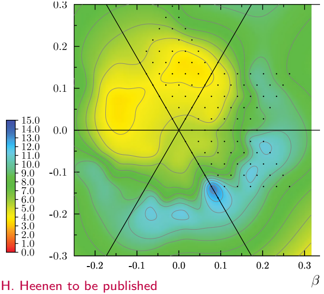
seniority 0

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




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

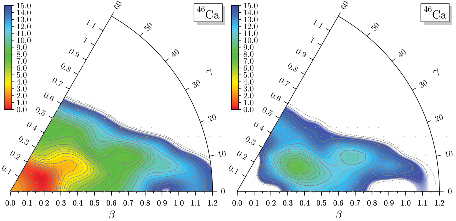



M. B.& P.-H. Heenen to be published

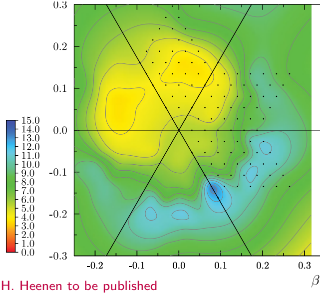
# Fun with SLyMR0 and diabatic states – $^{46}$Ca

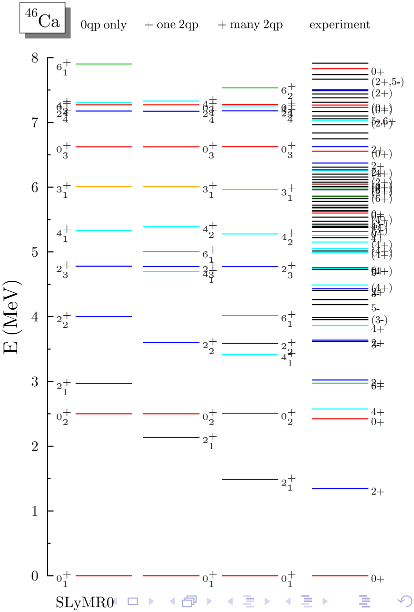
seniority 0

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




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




M. B.& P.-H. 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 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, M. B., PRC 88 (2013) 064326

- parameter fit is underway, leads to significantly improved phenomenology

# Take-away messages

- Many efforts 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 terms)
- projection on good quantum numbers restores selection rules for transitions
- configuration mixing (different shapes, different qp configurations, . . . )

**Pertinent ingredients for MR-EDF calculations**

B. Bally*
*CEA Saclay - ESNT, IRFU/Service de Physique Nucléaire, F-91191 Gif-sur-Yvette, France*

M. Bender†
*Université de Bordeaux, Centre d'Etudes Nucléaires de Bordeaux Gradignan, UMR5797, F-33175 Gradignan, France and*
*CNRS/IN2P3, Centre d'Etudes Nucléaires de Bordeaux Gradignan, UMR5797, F-33175 Gradignan, France*

T. Duguet‡
*CEA Saclay, IRFU/Service de Physique Nucléaire, F-91191 Gif-sur-Yvette, France*
*KU Leuven, Instituut voor Kern- en Stralingsfysica, 3001 Leuven, Belgium and*
*National Superconducting Cyclotron Laboratory and Department of Physics and Astronomy,*
*Michigan State University, East Lansing, MI 48824, USA*

Workshop of the *Espace de Structure et de réactions Nucléaires Théoriques*

to be held here at hopefully happier times in 2016

# 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 |

analysis of formal aspects

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

code development and benchmarking

| | |
|---|---|
| Benoît Avez | CEN Bordeaux Gradignan |
| Benjamin Bally | CEN Bordeaux Gradignan, now SPhN, CEA Saclay |
| Veerle Hellemans | Université Libre de Bruxelles |

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