

# Symmetry-restored multi-reference mean-field theory for nuclei

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Workshop on  
"Near-degenerate systems in nuclear structure and quantum chemistry  
from ab-initio many-body methods"  
Espace de Structure Nucléaire Théorique, Saclay, 2 April 2015



## Bottom lines

- ▶ I use old-school phenomenological effective interactions (energy density functionals (EDFs)) – no *ab-initio* in this talk!
- ▶ I will not worry about getting *in-medium* correlations from a "bare" Hamiltonian.
- ▶ I will address nuclear structure phenomena that require multi-reference techniques. (It turns out that almost all do!)

## Topics

- ▶ Why MR?
- ▶ From simple to increasingly complicated MR schemes.
- ▶ Technical issues.

## Semantics

- ▶ single reference (SR)  $\equiv$  self-consistent mean field, "HF", "HFB"
- ▶ multi reference (MR)  $\equiv$  projection and/or Generator Coordinate Method

## Nuclear physics jargon 101

- ▶ static correlations: what one gets by symmetry-breaking mean field
  - ▶ HFB-type pairing
  - ▶ deformation (quadrupole, octupole, ...)
  - ▶ high angular-momentum (nuclear physics jargon: high-spin) states
- ▶ dynamical correlations: correlations from "going beyond the mean field"
  - ▶ Correlations from symmetry restoration
  - ▶ shape mixing (because of deformation softness and/or shape coexistence)
  - ▶ excited states (vibrations, ...)
  - ▶ restoration of angular-momentum, parity and isospin selection rules for electromagnetic and weak transitions

## Why worry?

- ▶ nuclei are self-bound systems  $\Rightarrow$  conserved quantum numbers
- ▶ most, if not all, nuclei exhibit shape coexistence Heyde & Wood, RMP83 (2011) 1467
- ▶ individual and various collective excitation modes on the same energy scale
- ▶ large amplitude collective motion

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

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

$K$  is the  $z$  component of angular momentum in the body-fixed frame.

Projected states are given by

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

$f_J(K)$  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  $|\text{MF}(\mathbf{q})\rangle$  differing in a set of collective and single-particle coordinates  $\mathbf{q}$

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

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

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

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

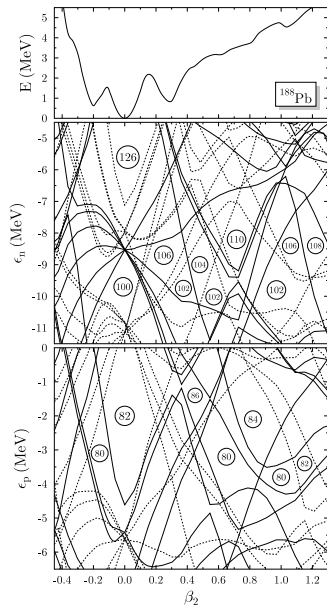
with

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

Angular-momentum projected GCM gives the

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

# Horizontal vs. vertical expansion of correlations



# Horizontal vs. vertical expansion of correlations

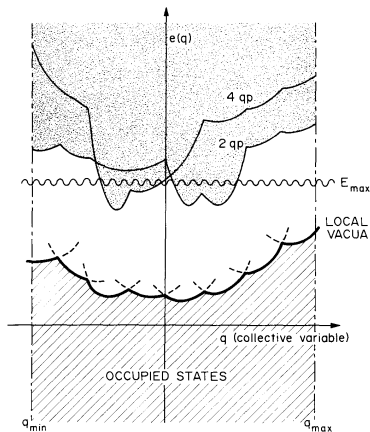
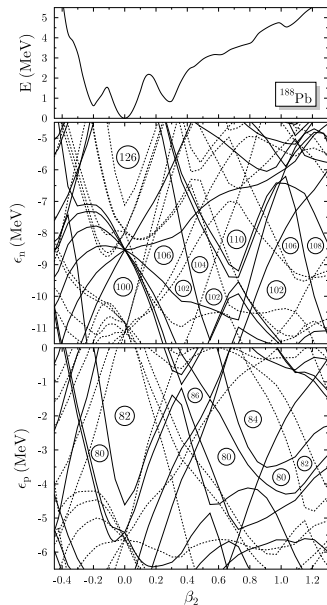


Fig. 1. Schematic plot of the energy versus the collective variable. The dark envelopes show the positions of the local vacua. The domain of the collective variable is defined by  $q_{\min}$ ,  $q_{\max}$  and the energy cut  $E_{\max}$ .

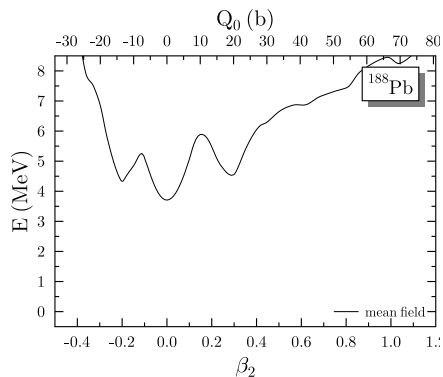
F. Dönau *et al*, NPA496 (1989) 333.

- ▶ Coordinate space representation on a 3d mesh using Lagrange-mesh techniques (in quantum chemistry jargon: a special case of a DVR)
- ▶ “HF+BCS” or “HFB” solved with two-basis method
- ▶ full space of occupied single-particle states
- ▶ Skyrme energy density functionals (old school) or Skyrme pseudo-potentials (new school)

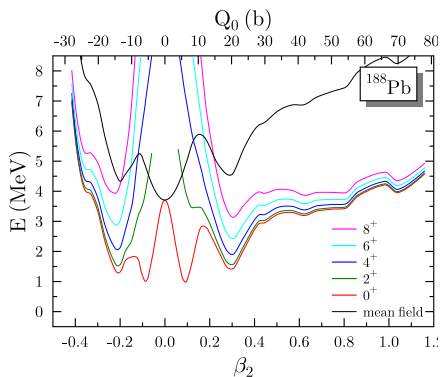


# Typical applications

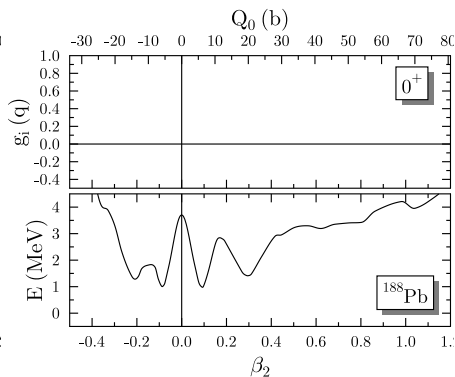
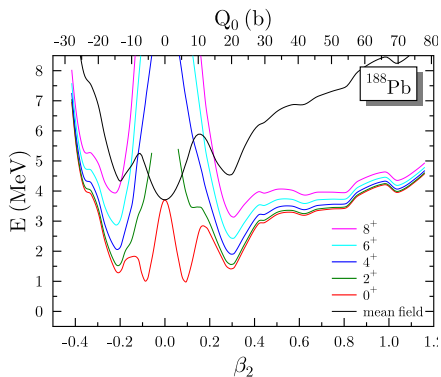
# Configuration mixing via the projected Generator Coordinate Method



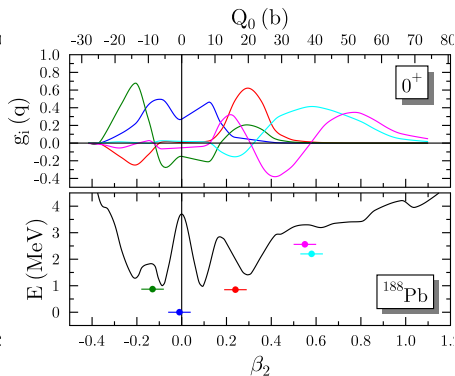
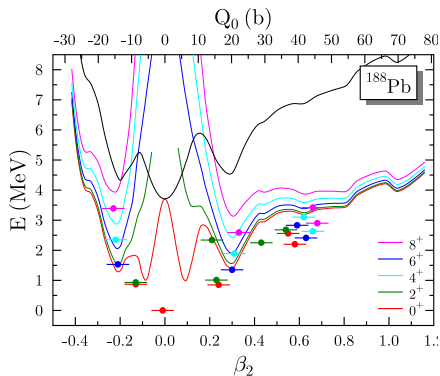
M. B., P. Bonche, T. Duguet, P.-H. Heenen, Phys. Rev. C 69 (2004) 064303.



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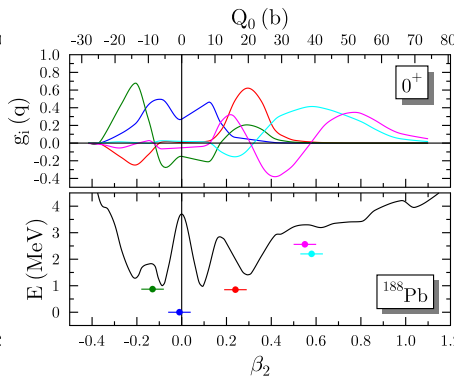
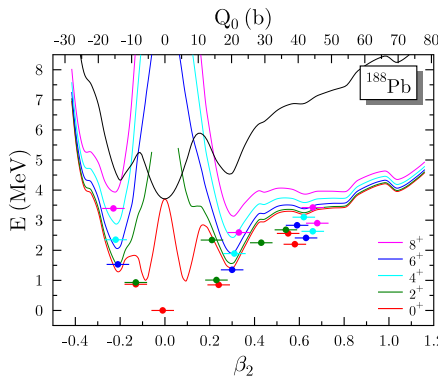


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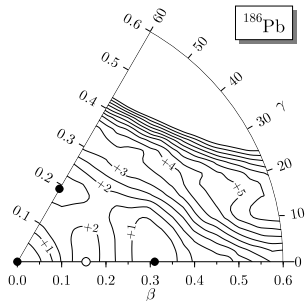
**Attention:**  $g_i^2(q)$  is not the probability to find a mean-field state with intrinsic deformation  $q$  in the collective state



M. B., P. Bonche, T. Duguet, P.-H. Heenen, Phys. Rev. C 69 (2004) 064303.

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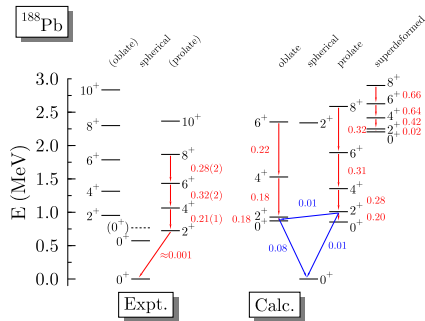
# Possible role of non-axial degrees of freedom



# Spectroscopy from MR EDF: Transition moments

M. B., P. Bonche, T. Duguet, P.-H. Heenen, Phys. Rev. C 69 (2004) 064303.

Experiment: T. Grahn et al, Phys. Rev. Lett. 97 (2006) 062501



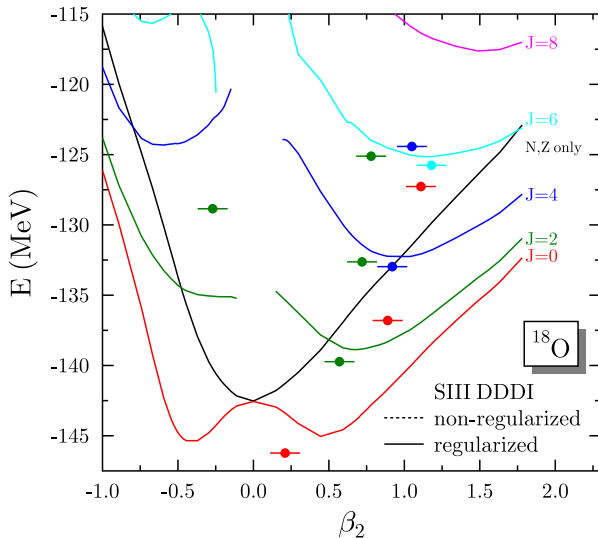
- ▶ in-band and out-of-band  $E2$  transition moments directly in the laboratory frame with correct selection rules
- ▶ full model space of occupied particles
- ▶ only occupied single-particle states contribute to the kernels ("horizontal expansion")
- ▶  $\Rightarrow$  no effective charges necessary
- ▶ no adjustable parameters

$$B(E2; J'_{\nu'} \rightarrow J_{\nu}) = \frac{e^2}{2J' + 1} \sum_{M=-J}^{+J} \sum_{M'=-J'}^{+J'} \sum_{\mu=-2}^{+2} |\langle JM\nu | \hat{Q}_{2\mu} | J'M'\nu' \rangle|^2$$

$$\beta_2^{(t)} = \frac{4\pi}{3R^2 A} \sqrt{\frac{B(E2; J \rightarrow J-2)}{(J020|(J-2)0)^2 e^2}} \quad \text{with} \quad R = 1.2 A^{1/3}$$

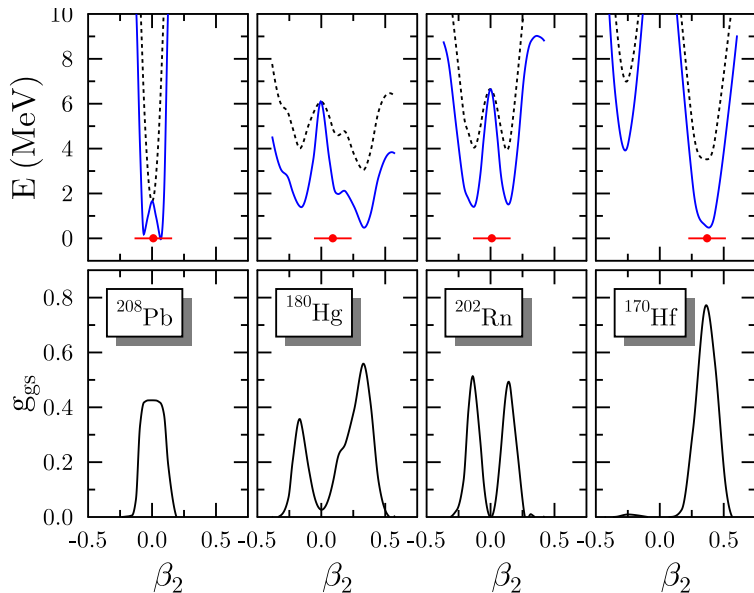


# Spherical nuclei don't stay spherical "beyond the mean field"

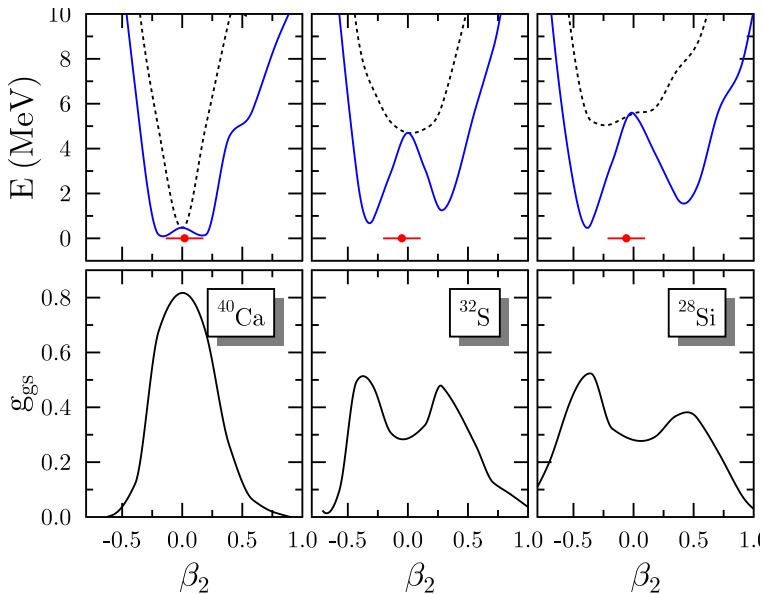


M. B., B. Avez, B. Bally, T. Duguet, P.-H. Heenen, D. Lacroix, unpublished

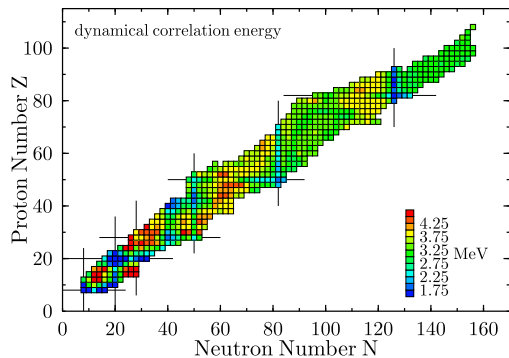
# Typical cases



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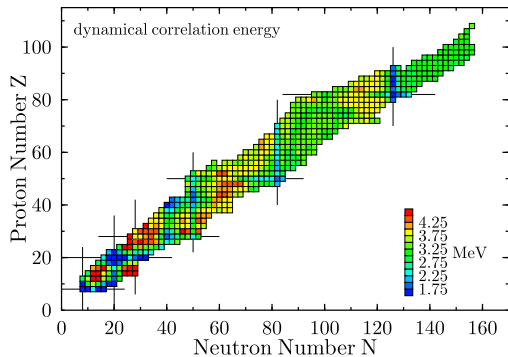


# Static vs. dynamical quadrupole correlation energies

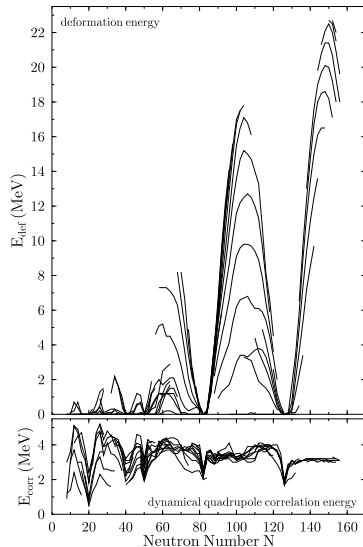


M. B., G. F. Bertsch, P.-H. Heenen, *Phys. Rev. C* 73 (2006) 034322

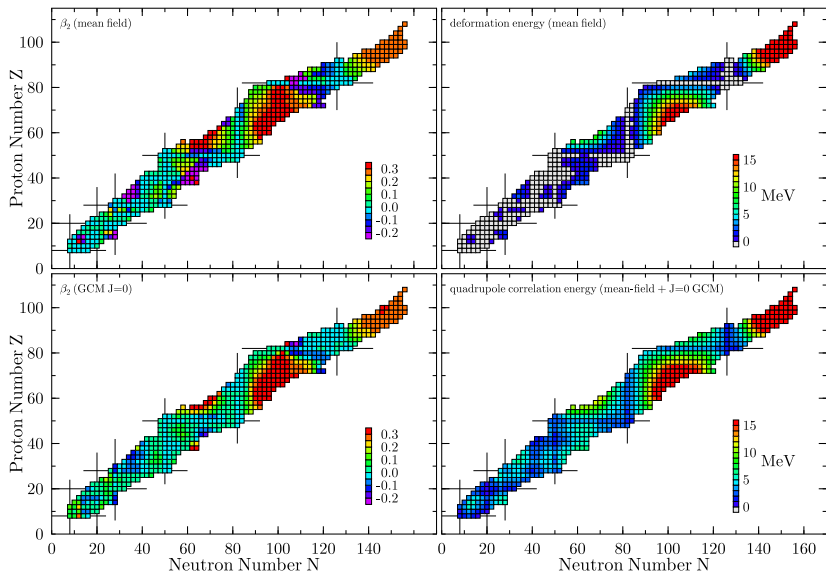
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M. B., G. F. Bertsch, P.-H. Heenen, *Phys. Rev. C* 73 (2006) 034322

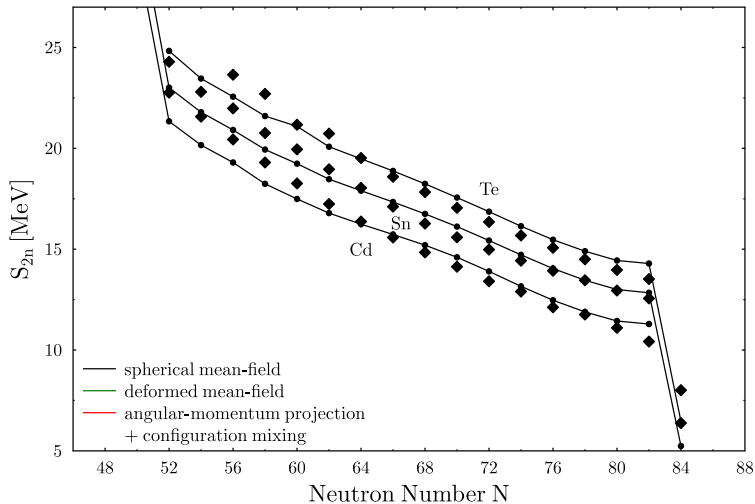


# Intrinsic Deformation and Quadrupole Correlation Energy



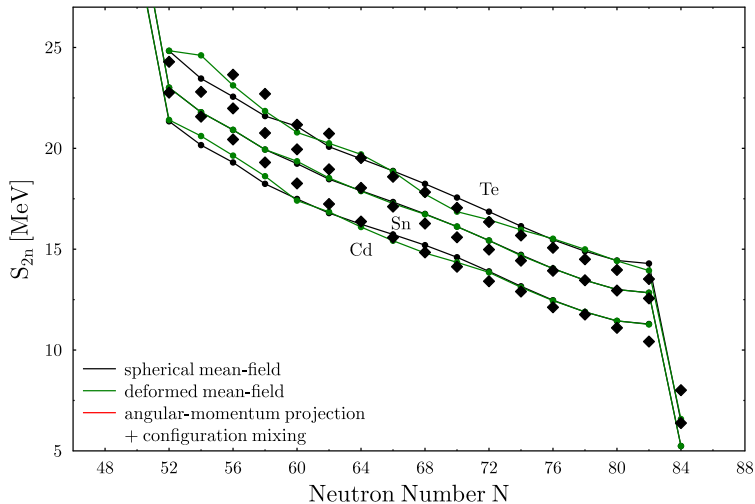
M. B., G. F. Bertsch, P.-H. Heenen, Phys. Rev. C 73 (2006) 034322

# Two-nucleon separation energies



data from M. B., G. F. Bertsch, P.-H. Heenen, Phys. Rev. C 73 (2006) 034322

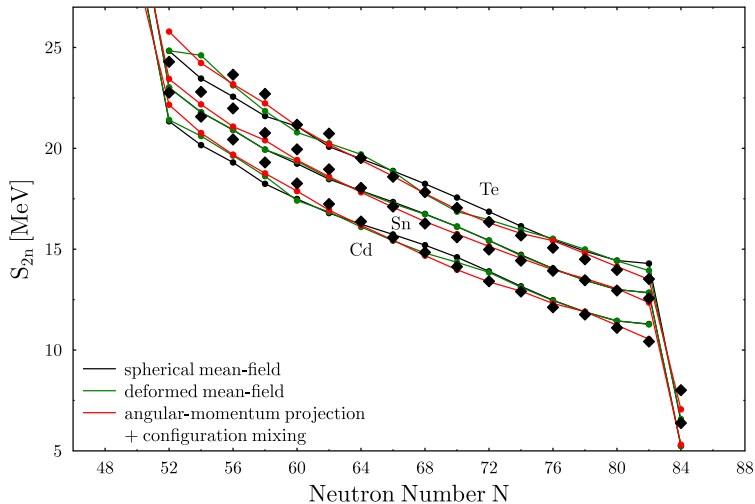
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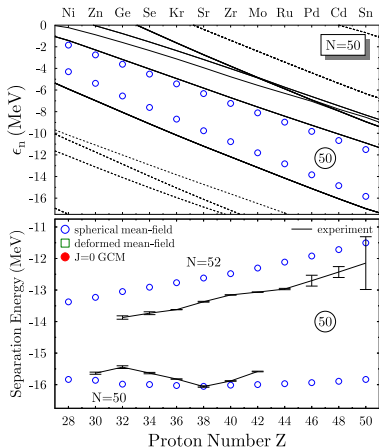
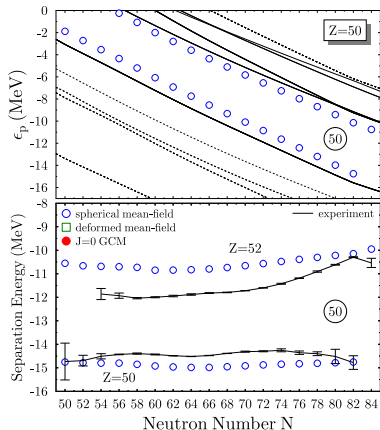


# Two-nucleon separation energies



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# 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  $S_{2p}$

M. B., G. F. Bertsch, P.-H. Heenen, PRC 78 (2008) 054312

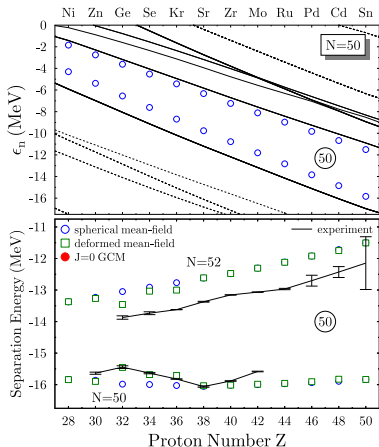
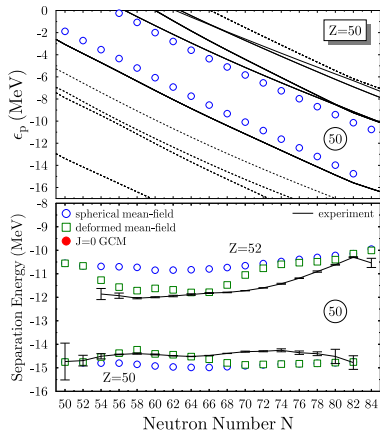
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M. B., G. F. Bertsch, P.-H. Heenen, PRC 78 (2008) 054312

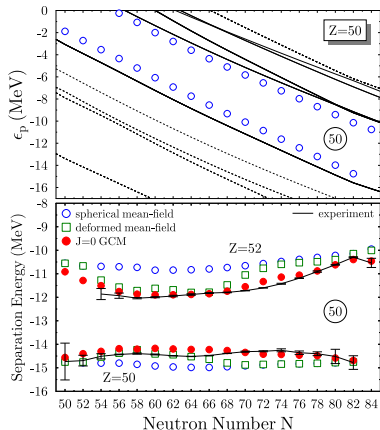
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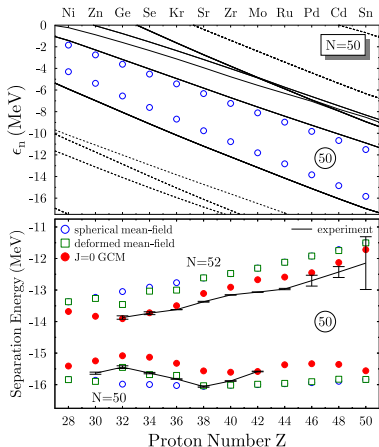
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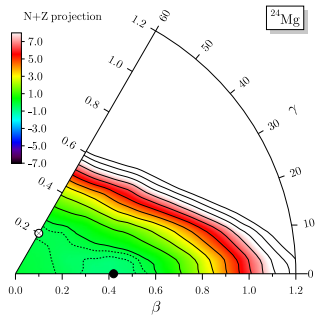
M. B., G. F. Bertsch, P.-H. Heenen, PRC 78 (2008) 054312



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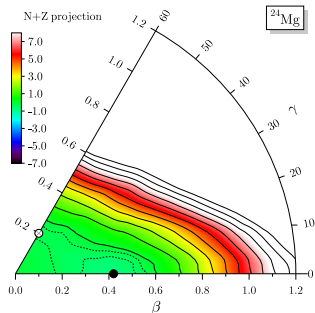
# Angular momentum projection of triaxial states

## mean-field deformation energy surface

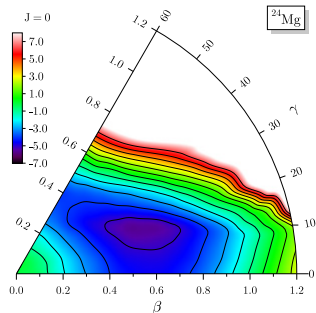


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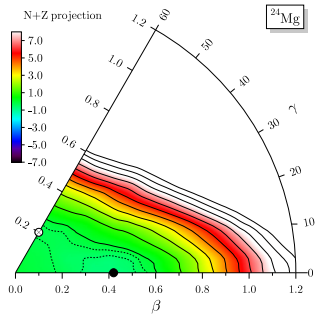


$J = 0$  projected deformation energy surface

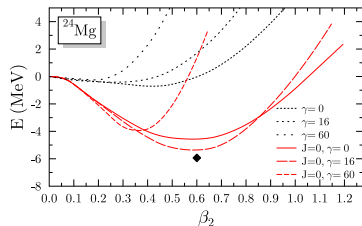
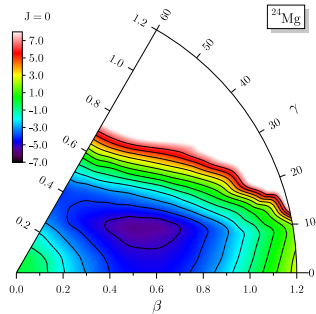


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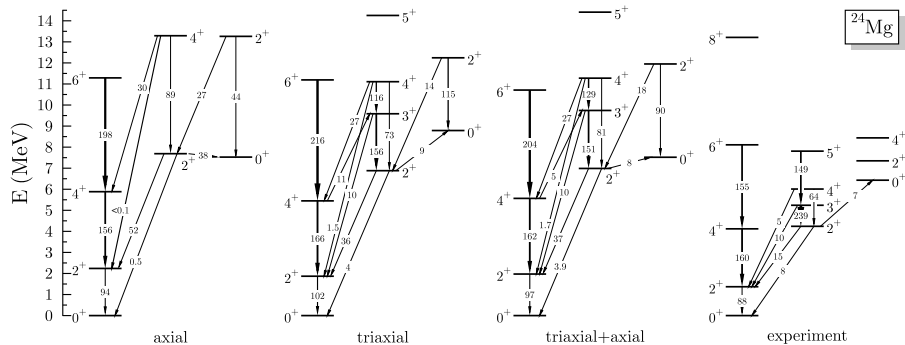
## mean-field deformation energy surface



## $J = 0$ projected deformation energy surface



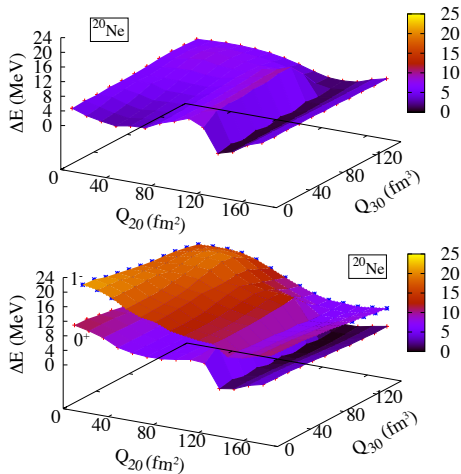
# Mixing of angular-momentum projected triaxial states of different intrinsic deformation



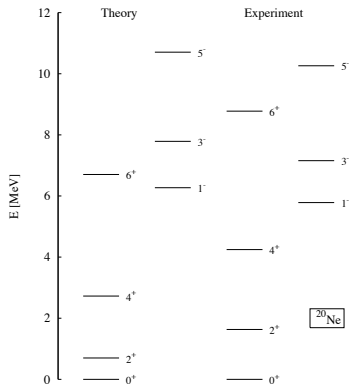
M. B. and P.-H. Heenen, Phys. Rev. C **78** (2008) 024309



# Other collective degrees of freedom: Octupole deformation

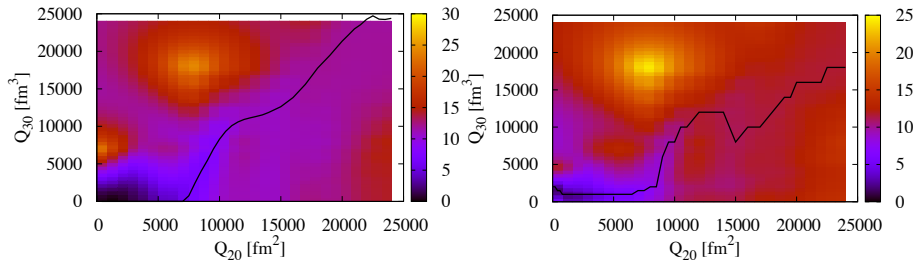


V. Hellemans, M. B., P.-H. Heenen, to be published.



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

# Towards the MR description of fission: the case of $^{180}\text{Hg}$



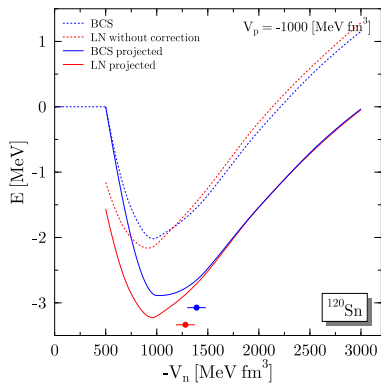
V. Hellemans, M. B., P.-H. Heenen, to be published.

- ▶ Skyrme SLy5s1 (recent parametrization with optimized surface tension) <sup>R</sup>.

Jodon, K. Bennaceur, M. B., J. Meyer, in preparation.

- ▶ axial states
- ▶  $N$ ,  $Z$ ,  $J$  & parity projection

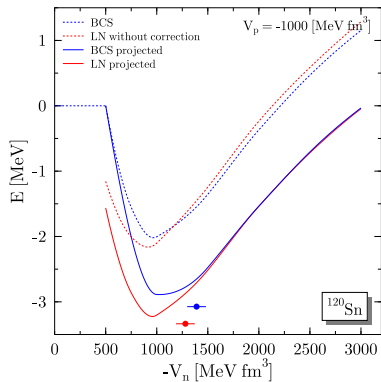
# Other collective degrees of freedom: dynamical pairing



Mixing of particle number projected spherical states in  $^{120}\text{Sn}$  with different amount of neutron pairing correlations

M. B., T. Duguet, IJMPE16 (2007) 222

# Other collective degrees of freedom: dynamical pairing



Mixing of particle number projected spherical states in  $^{120}\text{Sn}$  with different amount of neutron pairing correlations

M. B., T. Duguet, IJMPE16 (2007) 222

VAQUERO, EGIDO, AND RODRÍGUEZ

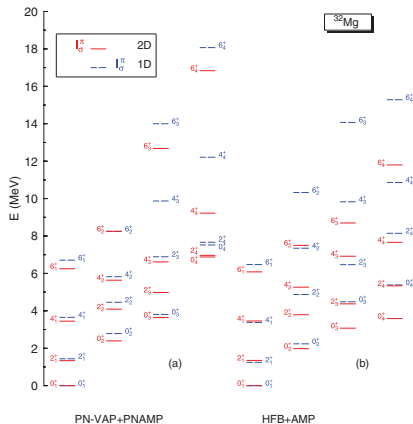


FIG. 12. (Color online) Spectra of  $^{32}\text{Mg}$  in the PN-VAP + PNAMP approach (left) and the HFB + AMP approach (right).

dynamical pairing combined with quadrupole GCM and projection on  $N$ ,  $Z$ , and  $J$

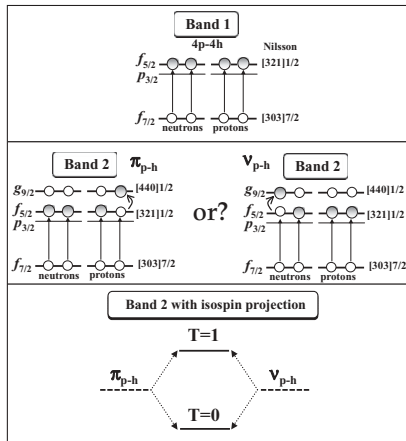
N. López Vaquero, J. L. Egido, T. R. Rodríguez, PRC 88 (2013) 064311

# Isospin breaking and restoration

isospin is a particular case:

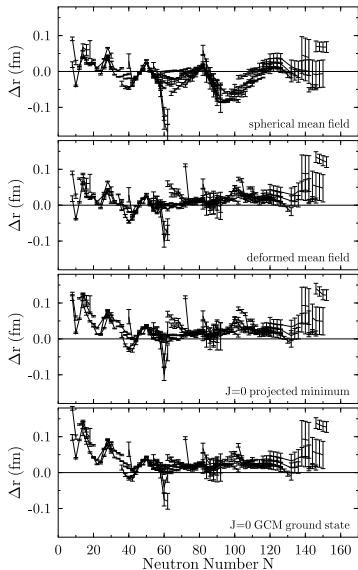
- ▶ physically broken by the Coulomb interaction, the difference of proton and neutron masses, and small contributions of the strong interaction
- ▶ spuriously broken by mean-field methods, with some severe consequences for calculated properties of nuclei close to the  $N = Z$  line.
- ▶ spurious breaking can be removed by diagonalizing the symmetry-breaking Hamiltonian in a basis of isospin-projected mean-field states.
- ▶ isospin projection mixes proton and neutron single-particle states.
- ▶ controlling the physical isospin breaking has relevance for tests of the standard model through the analysis of superallowed  $0^+ \rightarrow 0^+$  Fermi  $\beta$  decay

Example: rotational bands of  $^{56}\text{Ni}$

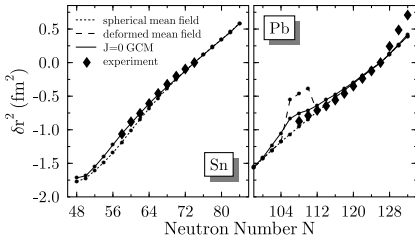


W. Satuła, J. Dobaczewski, W. Nazarewicz, M. Rafalski, PRC 81 (2010) 054310

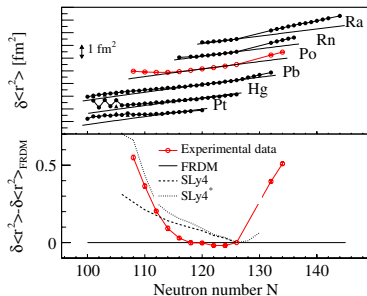
# charge radii: Experimental signatures of shape mixing



M. B., G. F. Bertsch, P.-H. Heenen, PRC 78 (2008) 054312

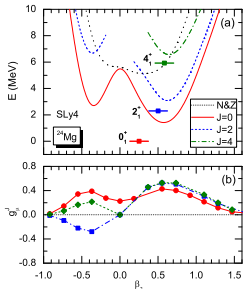


M. B., G. F. Bertsch, P.-H. Heenen, PRC 78 (2008) 054312

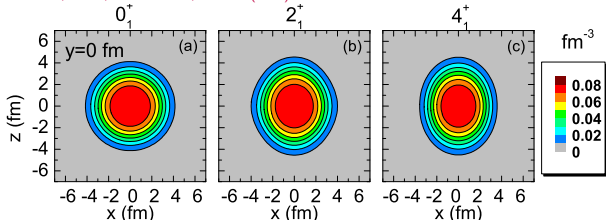


T. Cocolios, ..., M. B., P.-H. Heenen, PRL 106 (2011) 052503.

# Laboratory densities



J. M. Yao, M. B., P.-H. Heenen, PRC 91 (2015) 024301



Contour plots of the 3D proton densities (in  $\text{fm}^{-3}$ ) in the  $y=0$  plane for the  $0_1^+$  (a),  $2_1^+$  (b),  $4_1^+$  (c) states (with  $M=0$ ) in  $^{24}\text{Mg}$ .

Transition density in the laboratory between GCM states  $|J_i M_i \mu_i\rangle$  and  $|J_f M_f \mu_f\rangle$  assuming axial HFB states

$$\begin{aligned}
 \rho_{J_i M_i \mu_i}^{J_f M_f \mu_f}(\mathbf{r}) &= \sum_{qf, q_i} f_{\mu_f, q'}^{J_f} \langle q' | \hat{\rho}_{0M_f}^{J_f} \hat{\rho}(\mathbf{r}) \hat{\rho}_{0M_i}^{J_i \dagger} \hat{\rho}^N \hat{\rho}^Z | q \rangle f_{\mu_i, q}^{J_i 0} \\
 \text{with} \quad & \langle q' | \hat{\rho}_{0M_f}^{J_f} \hat{\rho}(\mathbf{r}) \hat{\rho}_{0M_i}^{J_i \dagger} \hat{\rho}^N \hat{\rho}^Z | q \rangle \\
 &= \frac{\hat{J}_f^2 \hat{J}_i^2}{(8\pi^2)^2} \int d\Omega' D_{0M_f}^{J_f*}(\Omega') \sum_K D_{K0}^{J_i}(\Omega') \int d\Omega'' D_{0K}^{J_i}(\Omega'') \langle q' | \hat{\rho}(\tilde{\mathbf{r}}_{\Omega'}) \hat{\rho}^N \hat{\rho}^Z \hat{R}^\dagger(\Omega'') | q \rangle \\
 &\equiv \frac{\hat{J}_f^2}{8\pi^2} \int d\Omega' D_{0M_f}^{J_f*}(\Omega') \sum_K D_{KM_i}^{J_i}(\Omega') \hat{R}^\dagger(\Omega') \rho_{q'q}^{J_f J_i K 0}(\mathbf{r})
 \end{aligned}$$

For the density of the GCM state  $|JM\mu\rangle$  one obtains

$$\rho_{JM\mu}^{JM\mu}(\mathbf{r}) = \sum_{qf, q_i} f_{\mu, q'}^{J*} f_{\mu, q}^{J0} \sum_{\lambda} Y_{\lambda 0}(\hat{\mathbf{r}}) \langle JM\lambda 0 | JM \rangle \sum_K \langle J0\lambda K | JK \rangle \int d\hat{\mathbf{r}}' \rho_{q'q}^{JK0}(r, \hat{\mathbf{r}}') Y_{\lambda K}^*(\hat{\mathbf{r}}')$$

# Recent developments



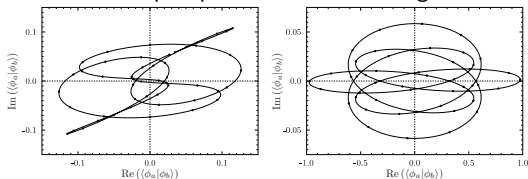
# Sign problem (of the overlap)

Onishi's formula:  $\langle q|q' \rangle^2 = \det(D)$  ( $\Rightarrow$  undetermined sign)

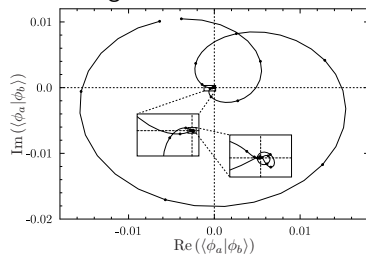
Starting point: L. Robledo, PRC 79 (2009) 021302; PRC 84 (2011) 014307:  
calculate overlap in some special cases from Pfaffian

Examples: 3d  $J$  projection:  $\alpha, \beta$  held fixed at some values,  $\gamma$  varied

one-quasiparticle states in  $^{25}\text{Mg}$



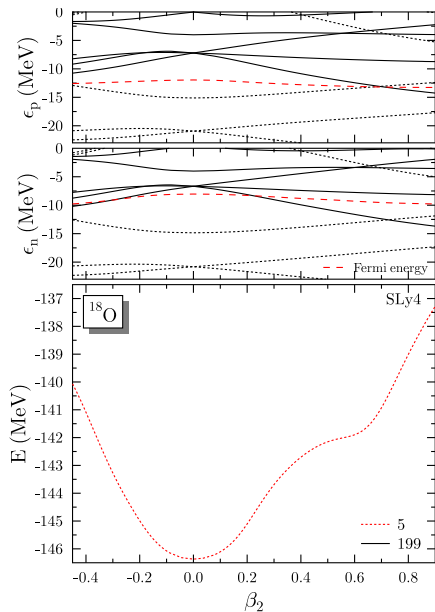
$^{24}\text{Mg}$  cranked to  $I = 8\hbar$



B. Avez & M. B., PRC 85 (2012) 034255

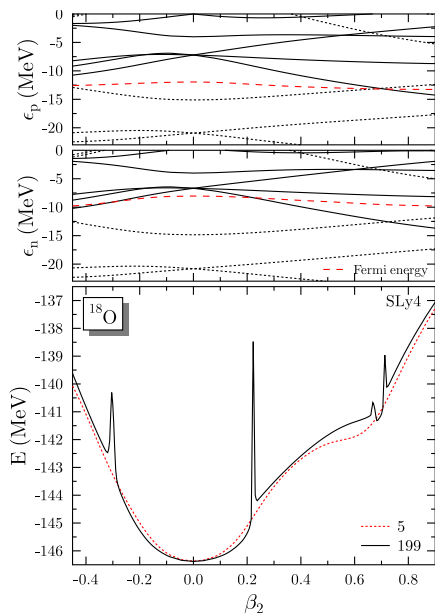
Similar expressions derived by Bertsch & Robledo, PRL108 (2012) 042505.

# "Pole problem"



► pure particle-number projection

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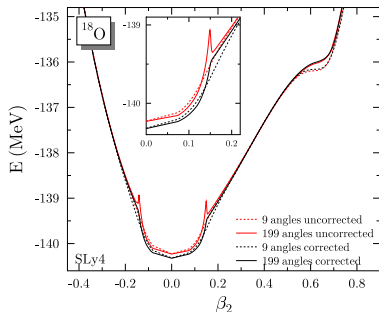


- ▶ pure particle-number projection
- ▶ first hints from Hamiltonian-based approaches in the form of failure of approximations: Dönau, PRC 58 (1998) 872; Almeded, Frauendorf, Dönau, PRC 63 (2001) 044311.
- ▶ analysis in density-dependent-Hamiltonian-based approach: Anguiano, Egido, Robledo NPA696 (2001) 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, Bender, PRC 79 (2009) 044318; Bender, Duguet, Lacroix, PRC 79 (2009) 044319; Duguet, Bender, Bennaceur, Lacroix, Lesinski, PRC 79 (2009) 044320; Bender, 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 termsthat 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

### Non-viability of non-integer density dependences



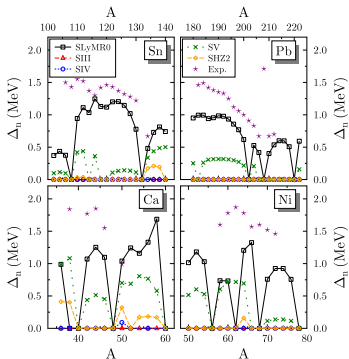
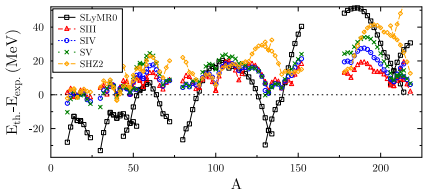
Duguet, Lacroix, M. B., Bennaceur, Lesinski, PRC 79 (2009) 044320

- ▶ in symmetry restored GCM, the local densities  $\rho^{qq'}(\mathbf{r})$  are in general complex
- ▶  $[\rho^{qq'}(\mathbf{r})]^\alpha$  is a multi-valued non-analytical function
- ▶ spurious contribution from branch cuts (see Dobaczewskiet *al.* PRC 76 (2007) 054315, and Duguet *et al.* PRC 79 (2009) 044320 for complex plane analysis)
- ▶ (partial) workaround when conserving specific symmetries: use particle-number projected densities for density dependence instead (strategy currently used by L. Egido and collaborators).
  - ▶ difficult to justify formally.
  - ▶ leads to unphysical excitation spectra when using time-reversal-invariance breaking reference states.

1. construct the EDF from a density-dependent Hamiltonians with special *ad-hoc* treatment of the density entering the density-dependent terms for which numerically efficient high-quality parameterizations can be easily constructed. Problem: cannot be defined for all possible configuration mixings of interest [Robledo, J. Phys. G 37 (2010) 064020] and/or fails when breaking time-reversal invariance [Bender, Avez, Bally, Heenen, in preparation].
2. 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]. Problems: complicated formalism. Almost works sometimes. Sometimes fails spectacularly.
3. constructing the EDF as expectation value of a strict Hamiltonian. New problems: numerically much more 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 with density-dependent coupling constants in the 1970s).

# Toy Skyrme Hamiltonian: SLyMR0

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



- ▶ impossible to fulfill 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

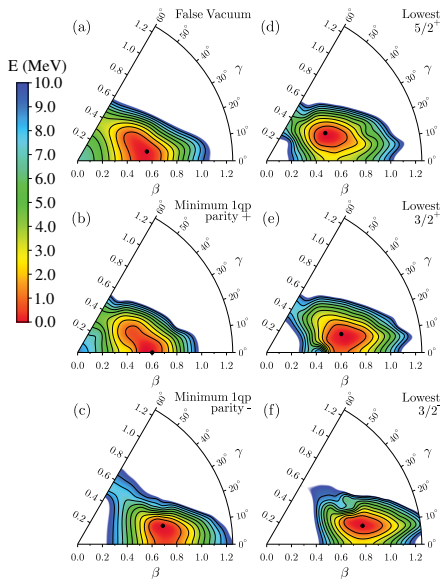
Nuclear physics jargon: breaking time-reversal invariance of the reference states

- ▶ one non-paired nucleon: odd- $A$  nuclei
- ▶ one or several broken pairs: states with seniority  $\neq 0$  (and usually  $J \neq 0$ ) in even-even nuclei
- ▶ disturbed pairs: angular-momentum optimized collectively rotating states (in nuclear physics jargon: self-consistent cranking)

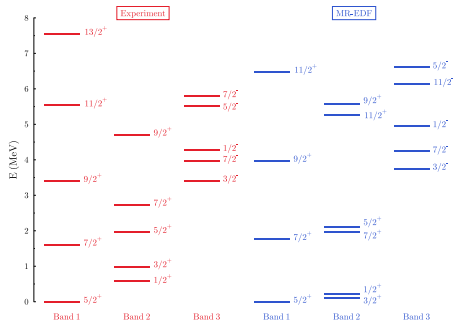
$$\hat{H} \rightarrow \hat{H} - \omega \cdot \hat{\mathbf{J}}$$



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



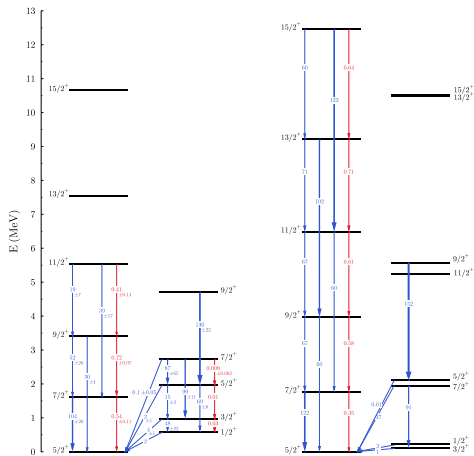
## Angular-momentum and particle-number projected GCM of blocked triaxial one-quasiparticle states



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

B. Bally, B. Avez, M. B., and P.-H. Heenen, PRL 113 (2014) 162501

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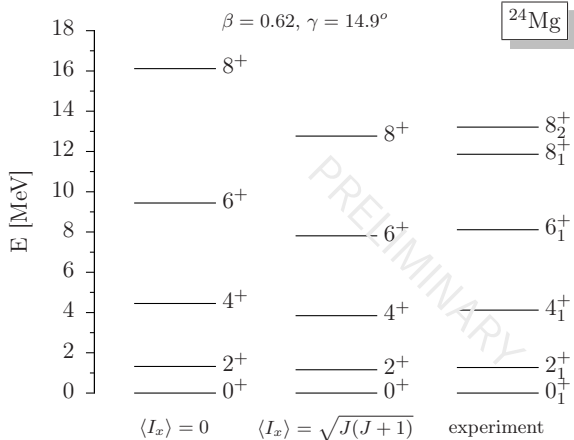


- ▶ spectroscopic quadrupole moment  $Q_s$  of the  $5/2^+$  ground state:  
Exp:  $20.1 \pm 0.3 e fm^2$   
Calc:  $23.25 e fm^2$
- ▶ magnetic moment  $\mu$  of the  $5/2^+$  ground state in nuclear magnetons:  
Exp:  $-0.855$   
Calc:  $-1.054$

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

Data from Nuclear Data Sheets 110 (2009) 1691

# Projection of cranked states



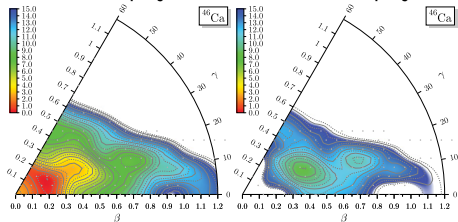
B. Bally, B. Avez, M. B., P.-H. Heenen (unpublished)

- ▶ compression of excitation spectrum
- ▶ projecting the states cranked to  $I$  does not lead to the lowest energy for  $J = I$  states.

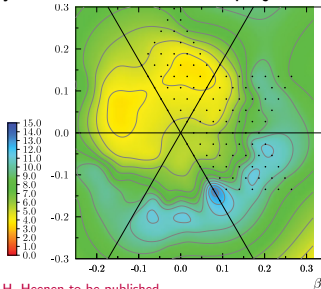
# MR EDF with diabatic states: $^{46}\text{Ca}$

seniority 0

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

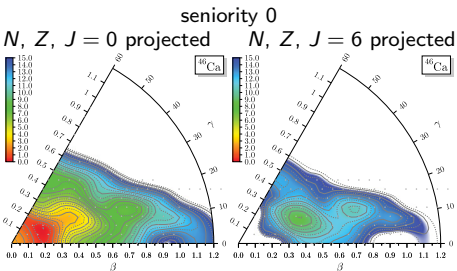


seniority 2, lowest  $N, Z, J = 6$  projected

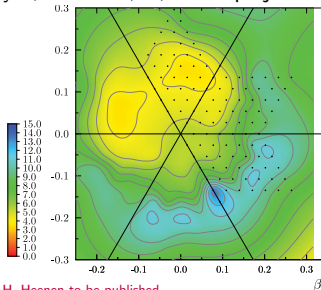


M. B. & P.-H. Heenen to be published

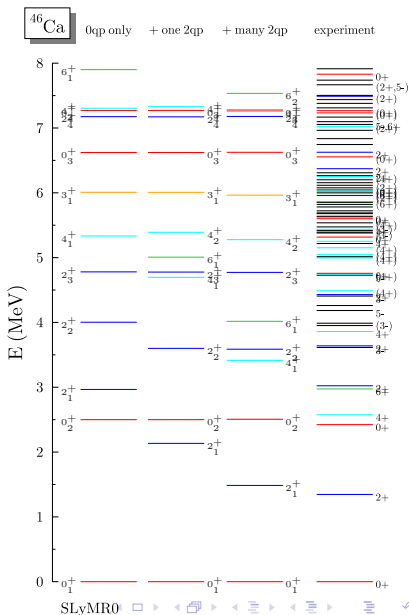
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M. B. & P.-H. Heenen to be published



- ▶ construction of most general central 3-body contact interaction of 2nd order in gradients [J. Sadoudi, T. Duguet, J. Meyer, M. B., PRC 88 \(2013\) 064326](#)
- ▶ parameter adjustment of a standard 2-body + central 3-body contact interaction up to 2nd order in gradients: SLyMR1 [R. Jodon, Thesis, Lyon \(2014\)](#). Better than SLyMR0, but still serious deficiencies.
- ▶ construction of most general spin-orbit + tensor 3-body force of 2nd order in gradients has been started by J. Sadoudi.

## What to add?

- ▶ two-body contact terms of 4th (and even 6nd) order in gradients
  - [F. Raimondi, B. G. Carlsson, J. Dobaczewski, J. Toivanen PRC84 \(2011\) 064303](#)
  - [D. Davesne, A. Pastore, J. Navarro, JPG 40 \(2013\) 095104](#)
  - [P. Becker, D. Davesne, J. Meyer, A. Pastore, J. Navarro, JPG 42 \(2015\) 034001](#)
- ▶ non-local finite range two-body terms
  - [F. Raimondi, K. Bennaceur, J. Dobaczewski, JPG41 \(2014\) 055112](#)
- ▶ semi-contact three-body force
  - [D. Lacroix, K. Bennaceur, PRC91 \(2015\) 011302R](#)

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- ▶ semi-contact three-body force  
[D. Lacroix, K. Bennaceur, PRC91 \(2015\) 011302R](#)
- ▶ or try a different strategy altogether: explicit in-medium correlations from MBPT  
[T. Duguet, M. Bender, J.-P. Ebran, T. Lesinski, V. Somà, arXiv:1502.03672](#)

- ▶ MR techniques provide useful tools to describe correlations related to the finiteness and self-boundedness of atomic nuclei
- ▶ symmetry restoration of symmetry-breaking reference states
- ▶ GCM-type mixing of (symmetry-restored) states
- ▶ The last 10 years brought a huge step forward in the advancement of implementation of multi-dimensional MR techniques
- ▶ there are interesting formal problems that we just start to identify and understand, and that remain to be solved



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development and benchmarking of new functionals

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Dany Davesne

Robin Jodon

Jacques Meyer

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