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

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Program on "Computational and Theoretical Advances for Exotic Isotopes in the Medium Mass Region" (INT-13-1a)
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Overview

Long-term goal:

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

Methodology:

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

Who are we?

The collaboration:

- B. Avez, B. Bally, M. Bender, J. Sadoudi
  CEN Bordeaux Gradignan, France
  formalism; beyond-mean-field models; construction of effective interactions; large-scale applications
- K. Bennaceur, D. Davesne, R. Jodon, J. Meyer
  IPN Lyon, France
  construction of effective interactions; parameter fit; nuclear matter
- T. Duguet
  SPhN / Irfu / CEA Saclay, France
  formalism; construction of effective interactions
- P.-H. Heenen, V. Hellemans, W. Ryssen
  Université Libre de Bruxelles, Belgium
  beyond-mean-field models, large-scale applications

Single-reference EDF: Some keywords

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

The standard Skyrme Energy Density Functional

$$
\begin{aligned}
\mathcal{E}_{\text{Skyrme}} \quad = \quad & \int d^3r \sum_{t=0,1} \Big\{ C_t^{\rho}[\rho_0]\,\rho_t^2 + C_t^{s}[\rho_0]\,\mathbf{s}_t^2 + C_t^{\Delta\rho}\rho_t\Delta\rho_t + C_t^{\tau}(\rho_t\tau_t - \mathbf{j}_t^2) \\
& + C_t^{T}\Big[\mathbf{s}_t\cdot\mathbf{T}_t - \sum_{\mu,\nu=x}^{z} J_{t,\mu\nu}J_{t,\mu\nu}\Big] + C_t^{\Delta s}\mathbf{s}_t\cdot\Delta\mathbf{s}_t \\
& + C_t^{F}\Big[\mathbf{s}_t\cdot\mathbf{F}_t - \tfrac{1}{2}\Big(\sum_{\mu=x}^{z} J_{t,\mu\mu}\Big)^2 - \tfrac{1}{2}\sum_{\mu,\nu=x}^{z} J_{t,\mu\nu}J_{t,\nu\mu}\Big] + C_t^{\nabla s}(\nabla\cdot\mathbf{s}_t)^2 \\
& + C_t^{\nabla\cdot J}(\rho_t\nabla\cdot\mathbf{J}_t + \mathbf{s}_t\cdot\nabla\times\mathbf{j}_t)\Big\}
\end{aligned}
$$

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

Local (transition) densities and currents

$$\rho_q(\mathbf{r}) = \sum_{ij} \frac{\langle \mathrm{L}|a_i^\dagger a_j|\mathrm{R}\rangle}{\langle \mathrm{L}|\mathrm{R}\rangle} \Psi_i^\dagger(\mathbf{r})\Psi_j(\mathbf{r})$$

$$\tau_q(\mathbf{r}) = \sum_{ij} \frac{\langle \mathrm{L}|a_i^\dagger a_j|\mathrm{R}\rangle}{\langle \mathrm{L}|\mathrm{R}\rangle} [\boldsymbol{\nabla}\Psi_i(\mathbf{r})]^\dagger \cdot \boldsymbol{\nabla}\Psi_j(\mathbf{r})$$

$$J_{q,\mu\nu}(\mathbf{r}) = -\tfrac{i}{2} \sum_{ij} \frac{\langle \mathrm{L}|a_i^\dagger a_j|\mathrm{R}\rangle}{\langle \mathrm{L}|\mathrm{R}\rangle} \{\Psi_i^\dagger(\mathbf{r})\, \sigma_\nu\, [\nabla_\mu \Psi_j(\mathbf{r})] - [\nabla_\mu \Psi_i(\mathbf{r})]^\dagger\, \sigma_\nu\, \Psi_j(\mathbf{r})\}$$

$$\mathbf{j}_q(\mathbf{r}) = -\tfrac{i}{2} \sum_{ij} \frac{\langle \mathrm{L}|a_i^\dagger a_j|\mathrm{R}\rangle}{\langle \mathrm{L}|\mathrm{R}\rangle} \{\Psi_i^\dagger(\mathbf{r})\, [\boldsymbol{\nabla}\Psi_j(\mathbf{r})] - [\boldsymbol{\nabla}\Psi_i(\mathbf{r})]^\dagger\, \Psi_j(\mathbf{r})\}$$

$$\mathbf{s}_q(\mathbf{r}) = \sum_{ij} \frac{\langle \mathrm{L}|a_i^\dagger a_j|\mathrm{R}\rangle}{\langle \mathrm{L}|\mathrm{R}\rangle} \Psi_i^\dagger(\mathbf{r})\, \hat{\boldsymbol{\sigma}}\, \Psi_j(\mathbf{r})$$

$$T_{q\mu}(\mathbf{r}) = \sum_{ij} \frac{\langle \mathrm{L}|a_i^\dagger a_j|\mathrm{R}\rangle}{\langle \mathrm{L}|\mathrm{R}\rangle} [\nabla\Psi_i(\mathbf{r})]^\dagger\, \hat{\boldsymbol{\sigma}}_\mu \cdot [\nabla\Psi_j(\mathbf{r})]$$

$$F_{q,\mu}(\mathbf{r}) = \tfrac{1}{2} \sum_{ij} \frac{\langle \mathrm{L}|a_i^\dagger a_j|\mathrm{R}\rangle}{\langle \mathrm{L}|\mathrm{R}\rangle} \{[\boldsymbol{\nabla}\cdot\hat{\boldsymbol{\sigma}}\Psi_i(\mathbf{r})]^\dagger\, [\nabla_\mu \Psi_j(\mathbf{r})] + [\nabla_\mu \Psi_i(\mathbf{r})]^\dagger\, [\boldsymbol{\nabla}\cdot\hat{\boldsymbol{\sigma}}\Psi_j(\mathbf{r})$$

For completeness: Other terms in the energy density functional

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

where

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

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

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

where there are two new "pairing densities"

$$\tilde{\rho}_q(\mathbf{r}) \equiv \sum_{ij} \frac{\langle \mathrm{L}|a_i a_j|\mathrm{R}\rangle}{\langle \mathrm{L}|\mathrm{R}\rangle} \sum_{\sigma=\pm 1} (-\sigma)\Psi_i(\mathbf{r},-\sigma)\Psi_j(\mathbf{r},\sigma)$$

$$\bar{\rho}_q^*(\mathbf{r}) \equiv \sum_{ij} \frac{\langle \mathrm{L}|a_i^\dagger a_j^\dagger|\mathrm{R}\rangle}{\langle \mathrm{L}|\mathrm{R}\rangle} \sum_{\sigma=\pm 1} (-\sigma)\Psi_i^*(\mathbf{r},\sigma)\Psi_j^*(\mathbf{r},-\sigma)$$

Symmetry restoration

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

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

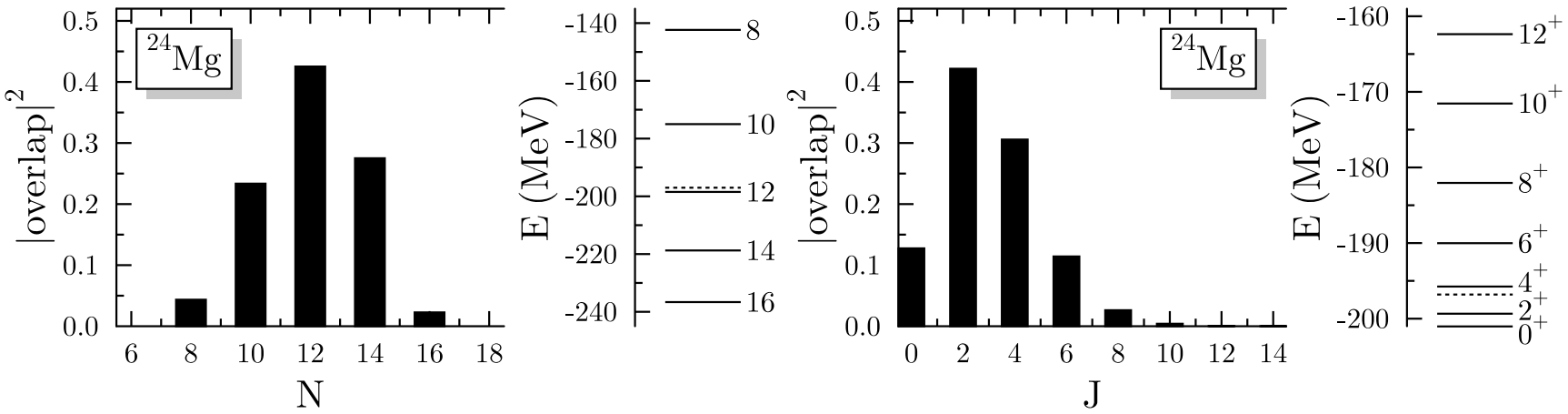
K is the z component of angular momentum in the body-fixed frame.
Projected states are given by

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

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

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

Symmetry restoration



Symmetry restoration schemes

- projection after variation (PAV): project mean-field minimum.
  - Advantage: simple
  - Problem: not variational. Unreliable in case of absent/weak static correlations
- variation after projection (VAP): vary projected state to determine the Slater determinant/HFB state that gives optimum projected state
  - Advantage: variational
  - Problem: expensive. existing codes for particle number and parity projection
- minimization after projection (MAP): generate set of mean-field states that differ in a collective coordinate that measures the amount of symmetry breaking, project them and search for the minimum of this energy curve/surface
  - Advantage: simple
  - Problem: not fully variational. Might fail if (projected) energy surface is soft in degrees of freedom that are not explicitely treated
- . . . or combine projection with a mixing of states that differ in a collective coordinate that measures the amount of symmetry breaking. This automatically includes the minimum of the projected energy curve/surface and additionally correlations not related to symmetry restoration

Configuration mixing by the symmetry-restored Generator Coordinate Method

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

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

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

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

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

with

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

Angular-momentum projected GCM gives the

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

Symmetry breaking and restoration

- Benefit: symmetries are broken on purpose: describes *n*p-*n*h and p-p shell-model correlations ("Jahn-Teller effect", pairing, ...) with a single product state at very modest computational cost
- Difficulty: scheme works only in the limits of neglible symmetry breaking and strong symmetry breaking, not in between.
- Price to pay: missing correlations related to symmetry restoration; difficult connection to the laboratory frame for spectroscopic observables; absence of selection rules for transitions
- Examples of broken symetries:

symmetry	quantum number	
translational	momentum	finite nuclei
rotational	angular momentum	deformed nuclei
space inversion	parity	octupole-deformed nuclei
gauge	particle number	paired systems

- symmetry restoration correponds to fluctuations within a set of degenerate product states differing by a "rotation"

Multi-reference energy density functional methods

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

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

$$E_q^{HFB} = \langle \mathrm{SR}_q | \hat{H} | \mathrm{SR}_q \rangle$$

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

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

- GCM: coherent superposition of Slater determinants/HFB states

$$\begin{aligned} |\mathrm{MR}_\mu\rangle &= \sum_q f_\mu(q) \, |\mathrm{SR}_q\rangle \\ \Rightarrow \quad E_\mu &= \langle \mathrm{MR}_\mu | \hat{H} | \mathrm{MR}_\mu \rangle = \sum_{q,q'} f_\mu^*(q) \, \langle \mathrm{SR}_q | \hat{H} | \mathrm{SR}_{q'} \rangle \, f_\mu(q') \end{aligned}$$

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

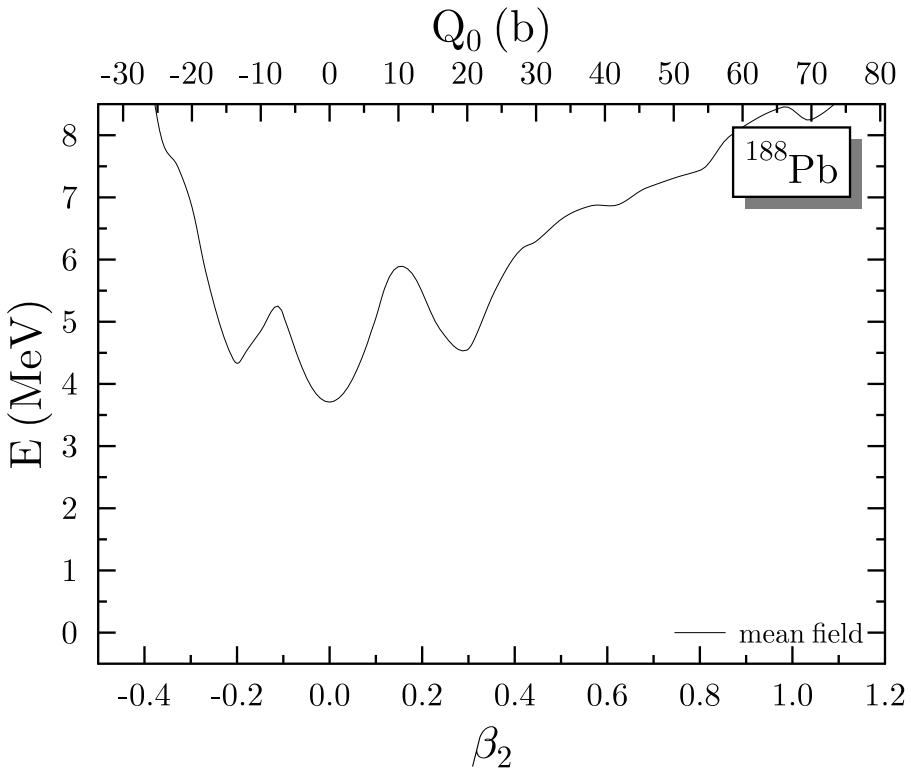
$$\mathcal{E}_\mu^{\mathrm{MR}} = \sum_{q,q'} f_\mu^*(q) \, \mathcal{E}_{qq'}^{\mathrm{MR}}[\rho_{qq'}, \kappa_{qq'}, \kappa_{qq'}^*] \, f_\mu(q') \quad \text{where} \quad \rho_{qq'} = \langle \mathrm{SR}_q | \hat{\rho} | \mathrm{SR}_{q'} \rangle$$

A few words on numerics: The Lagrange-mesh method

cf. the talk by Michael McNeil Forbes on monday, 8th april.
Nuclear structure codes that I am aware of using such techniques

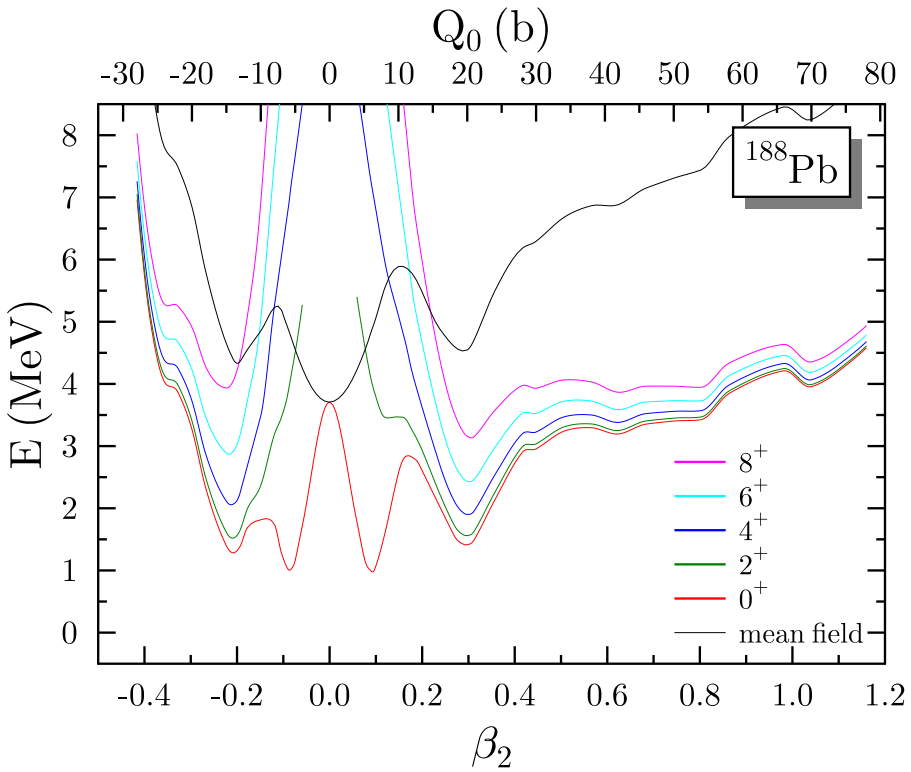
- V. Blum, G. Lauritsch, J. A. Maruhn, P.-G. Reinhard, J. Comp. Phys. 100 (1992) 364.
- 2d Skyrme relativistic mean-field code by V. Blum using FFT techniques (V. Blum, Doctoral Dissertation, J. W. Goethe-Universität Frankfurt am Main, 1992)
- 2d Skyrme HF+BCS code by P.-G. Reinhard using FFT techniques ($<$ 1994)
- spherical 1d, axial 2d, 3d relativistic mean-field codes by K. Rutz using FFT techniques (K. Rutz, Doctoral Dissertation, J. W. Goethe-Universität Frankfurt am Main, 1998)
- spherical 1d, axial 2d, 3d Skyrme HF+BCS codes based on Rutz's RMF codes (M. Bender, Doctoral Dissertation, J. W. Goethe-Universität Frankfurt am Main, 1998)
- Lagrange-mesh method (D. Baye & P.-H. Heenen, JPA 19 (1986) 2041)
- 3d cranked HF and angular-momentum projection using Lagrange-mesh methods (D. Baye & P.-H. Heenen, PRC 29 (1984) 1056)
- GCM kernels of symmetry-restored 3d HF+BCS states (A. Valor, P.-H. Heenen, P. Bonche, NPA 671 (2000) 145; M. Bender, P.-H. Heenen, PRC 78 (2008) 024309)

Configuration mixing via the projected Generator Coordinate Method



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

Milestones: Spectroscopy of heavy nuclei from MR EDF



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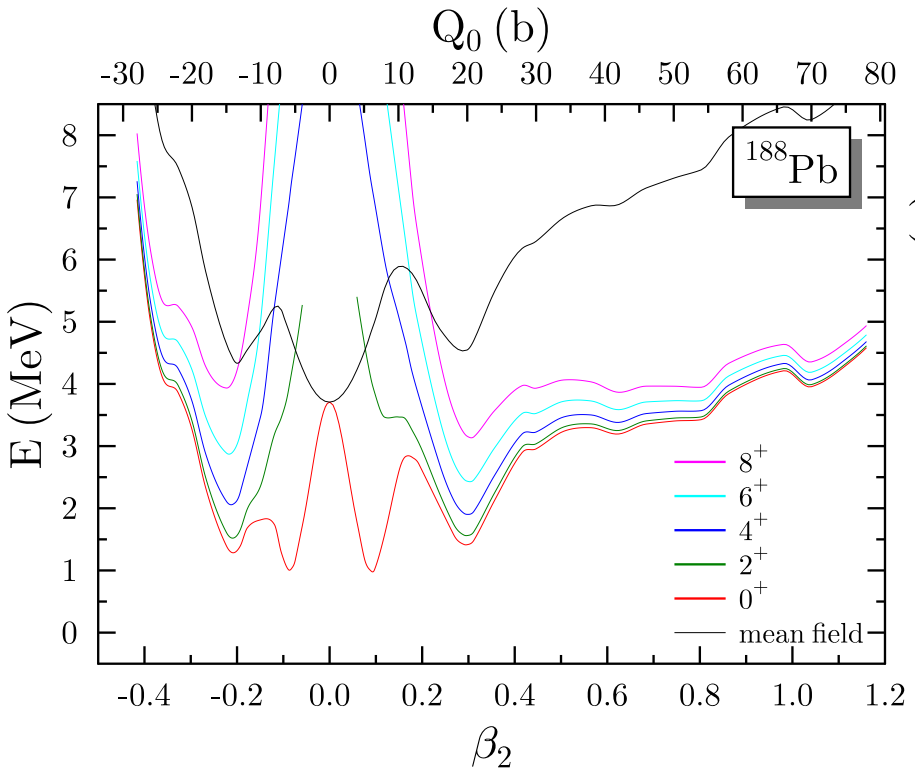

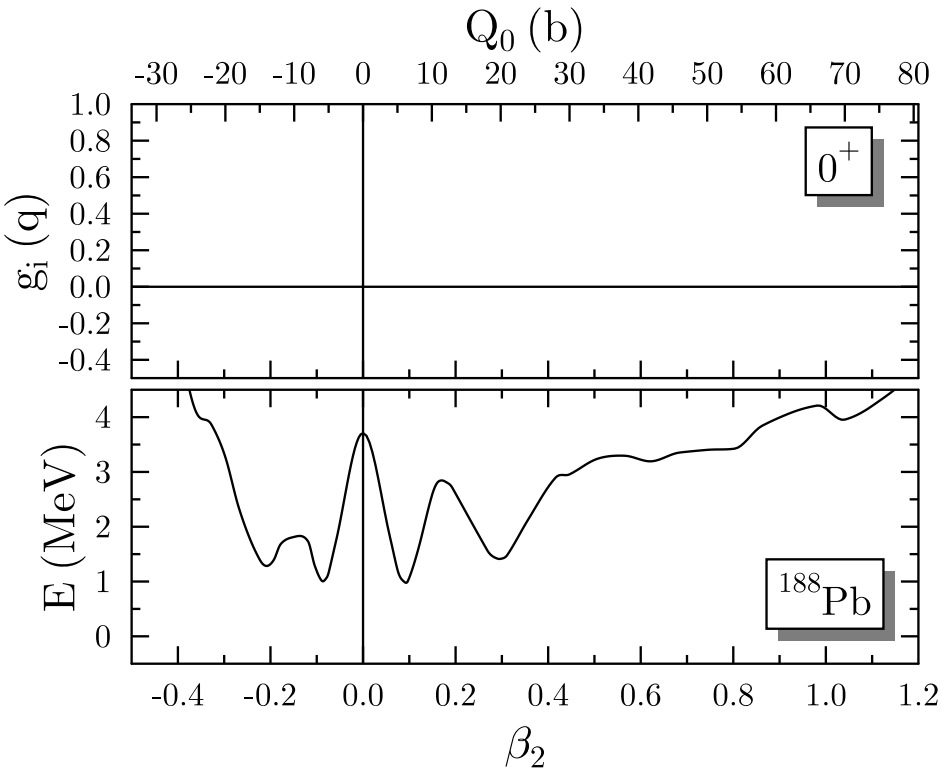

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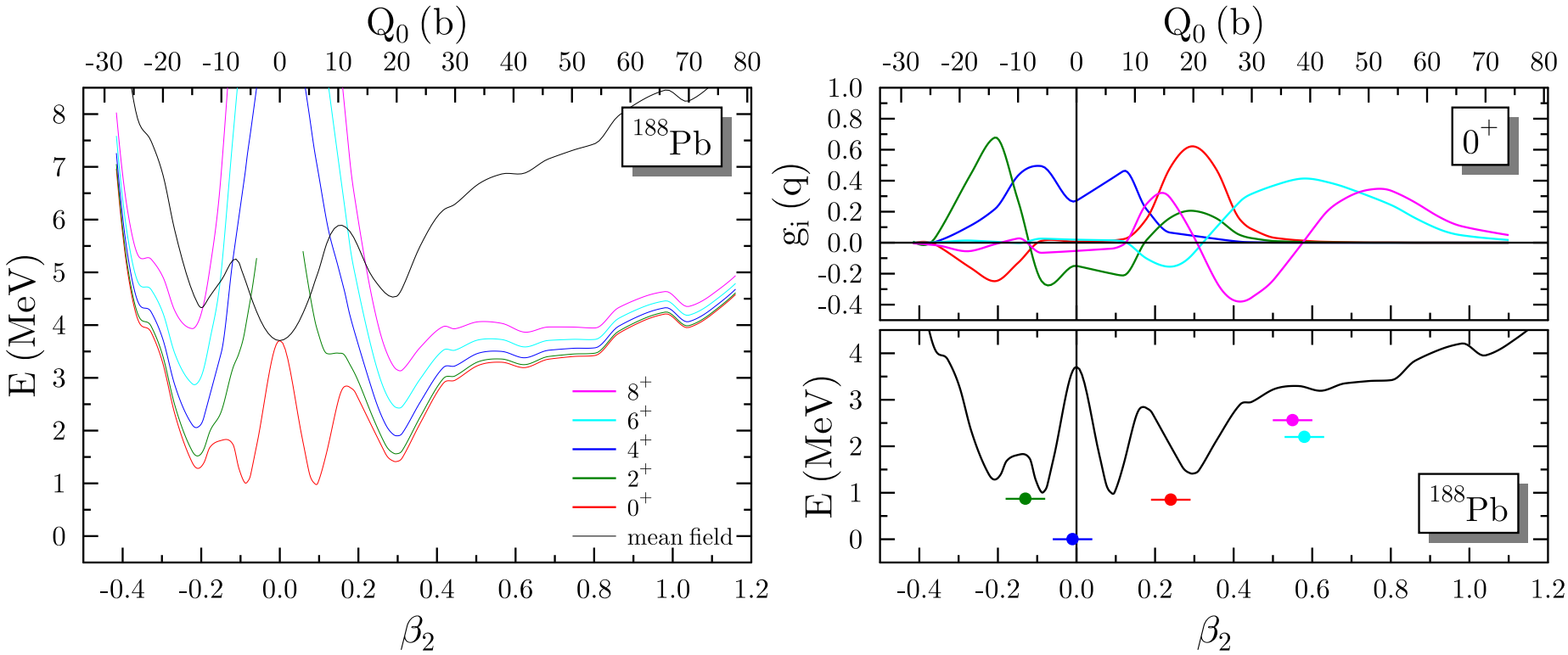

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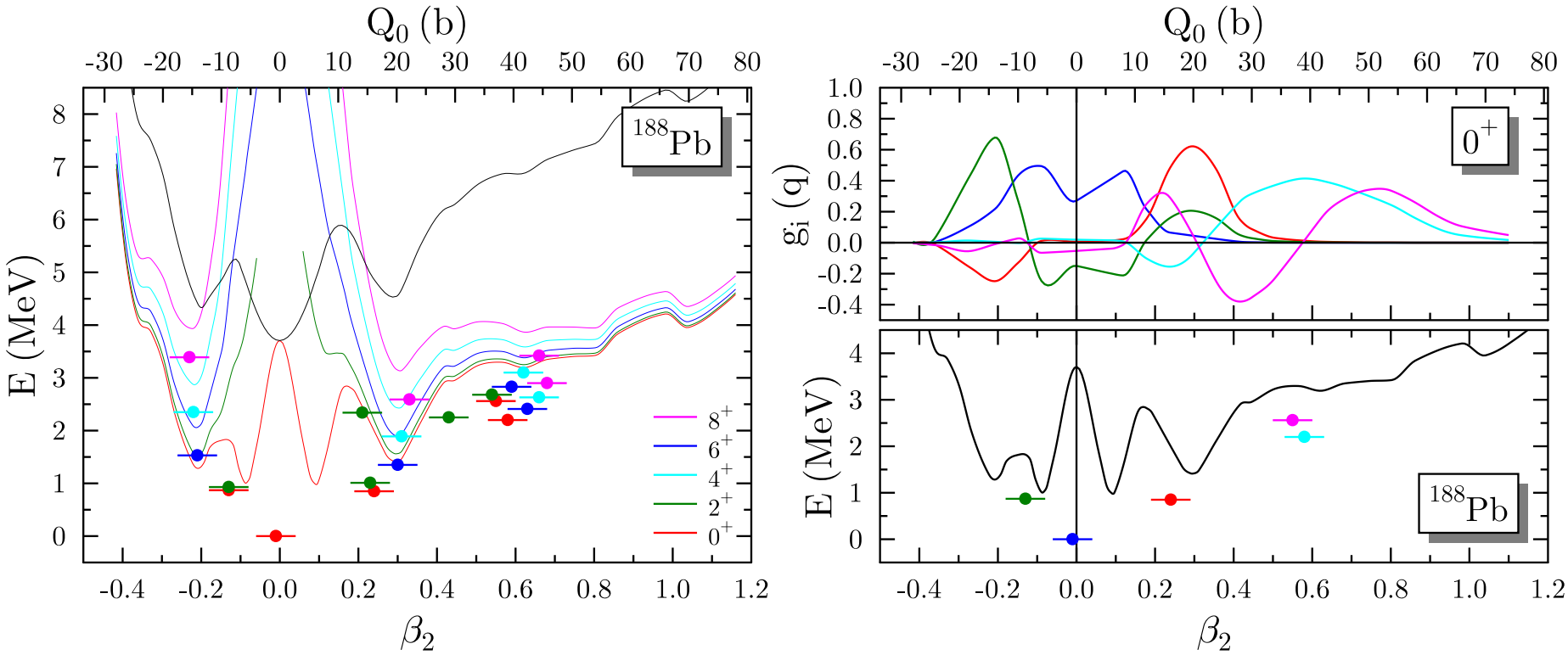
Attention: $g_i^2(q)$ is not the probability to find a mean-field state with intrinsic deformation q in the collective state

Milestones: Spectroscopy of heavy nuclei from MR EDF



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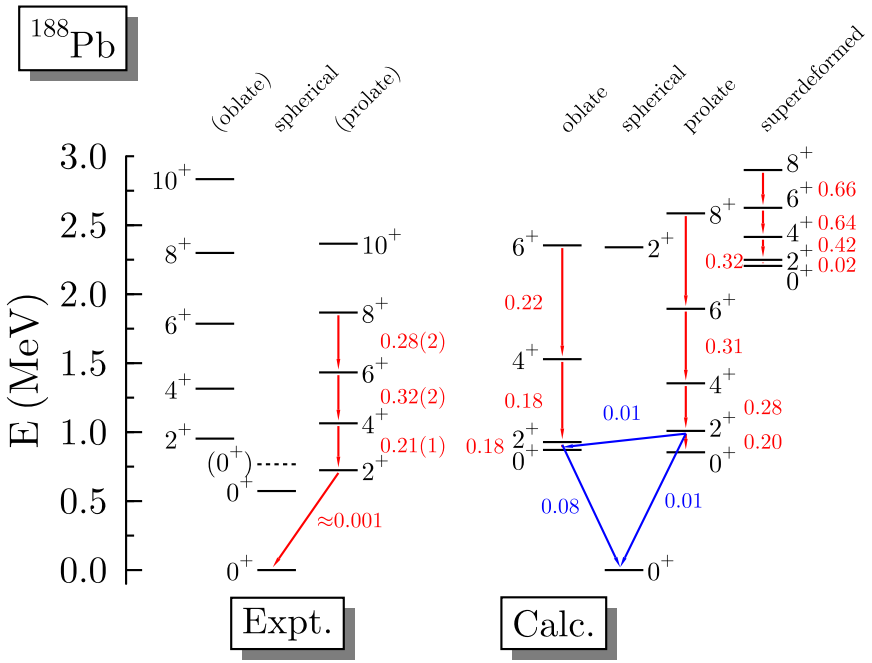
M. B., P. Bonche, T. Duguet, P.-H. Heenen, Phys. Rev. C 69 (2004) 064303.
Experiment: T. Grahn *et al*, Phys. Rev. Lett. **97** (2006) 062501

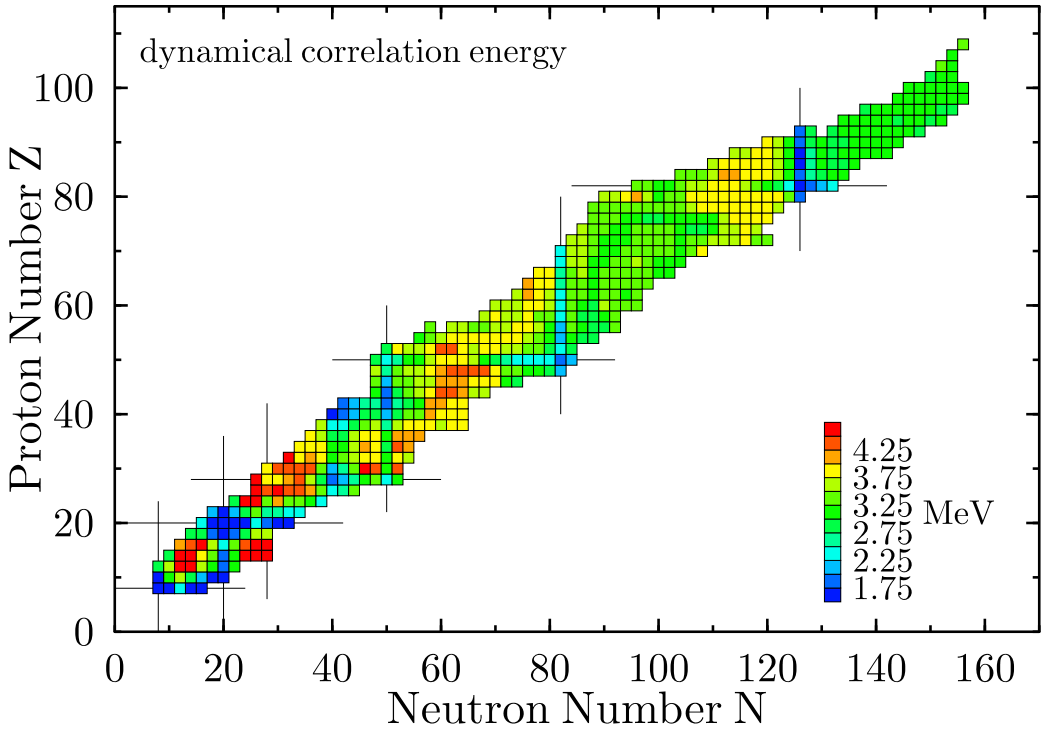


- in-band and out-of-band $E2$ transition moments directly in the laboratory frame with correct selection rules
- full model space of occupied particles
- only occupied single-particle states contribute to the kernels ("horizontal expansion")
- $\Rightarrow$ *no effective charges necessary*
- *no adjustable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

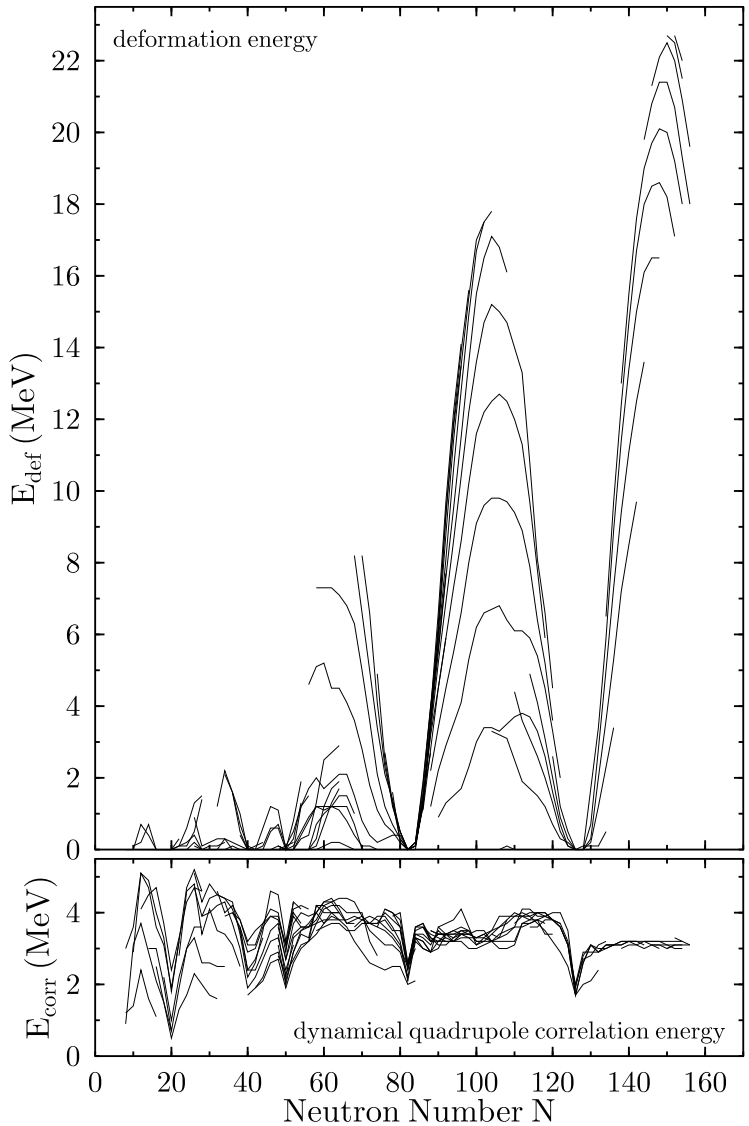
$$B(E2; J'_{\nu'} \to J_\nu) = \frac{e^2}{2J'+1} \sum_{M=-J}^{+J} \sum_{M'=-J'}^{+J'} \sum_{\mu=-2}^{+2} |\langle JM\nu|\hat{Q}_{2\mu}|J'M'\nu'\rangle|^2$$

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

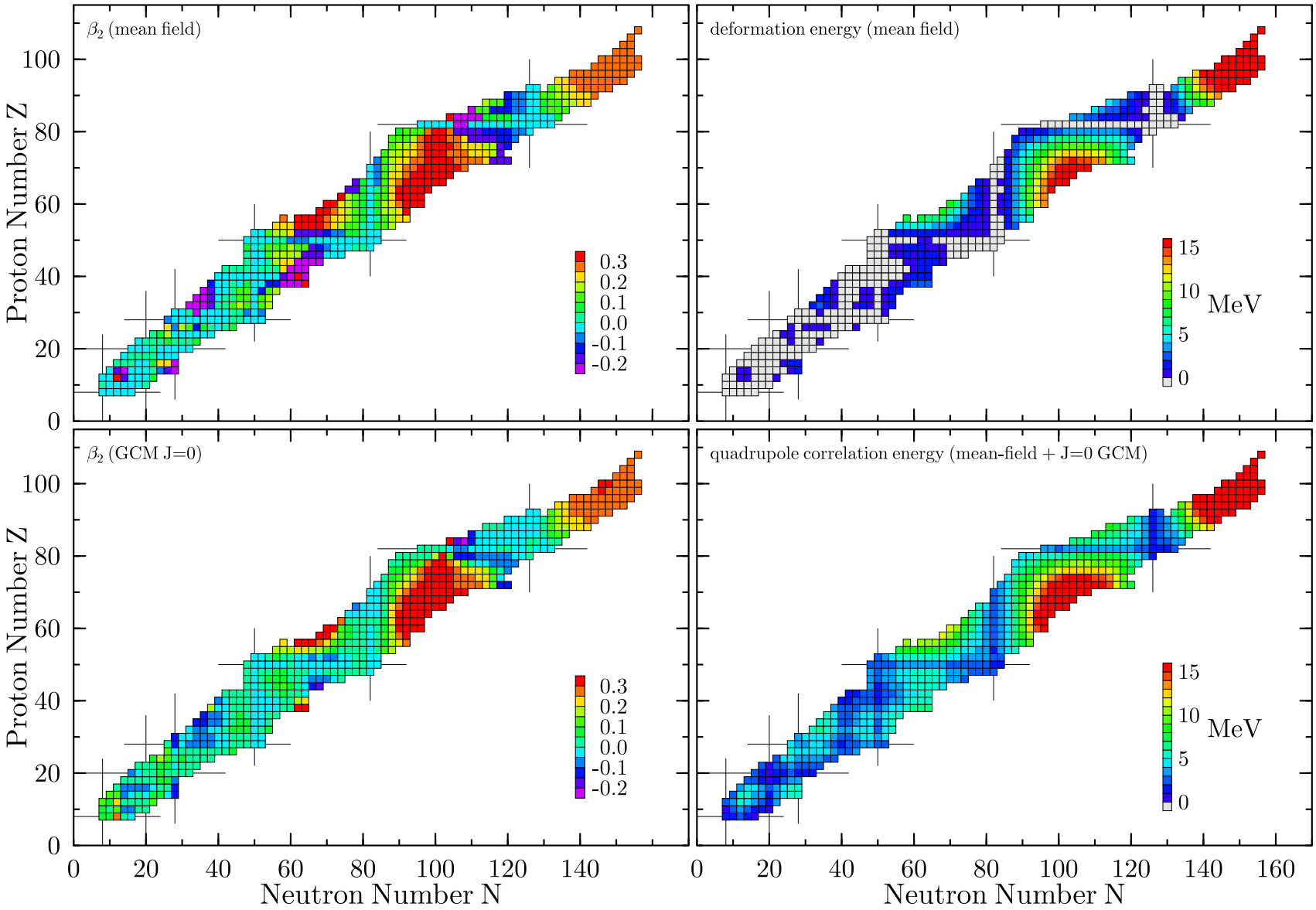
Static and Dynamic Quadrupole Correlation Energies



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



Intrinsic Deformation and Quadrupole Correlation Energy



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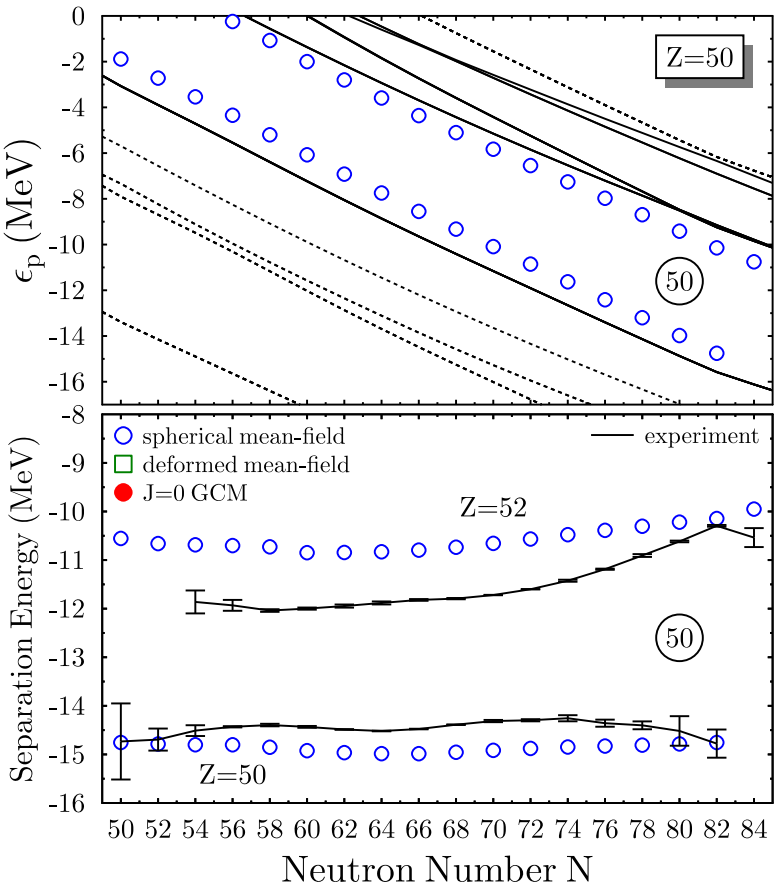
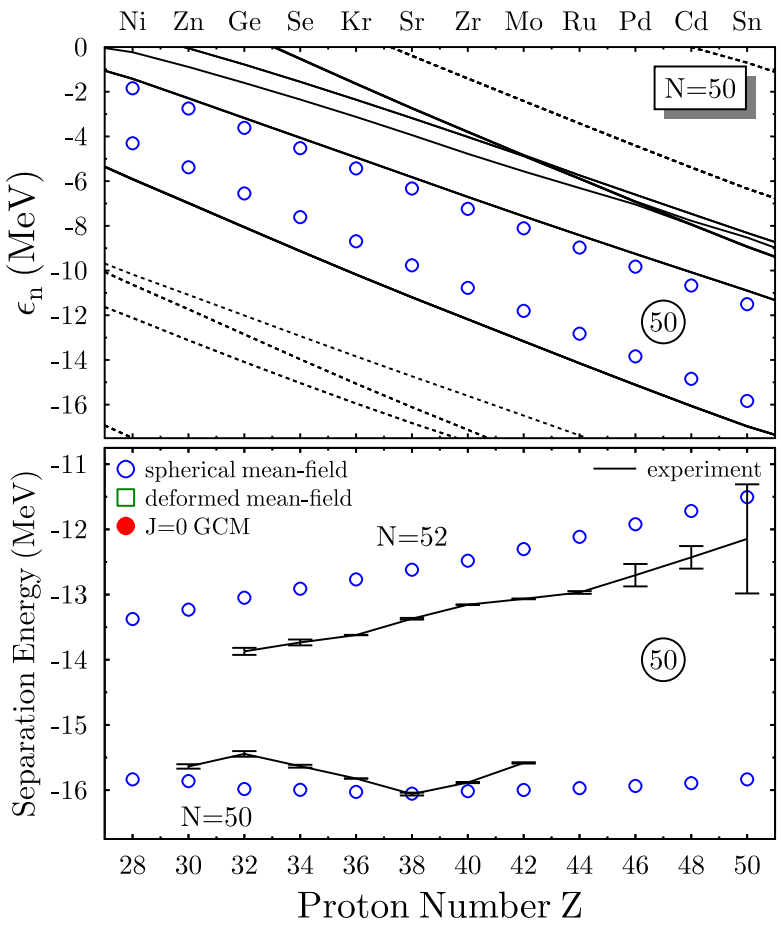
Eigenvalues of the single-particle Hamiltonian vs. S_{2q}





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}

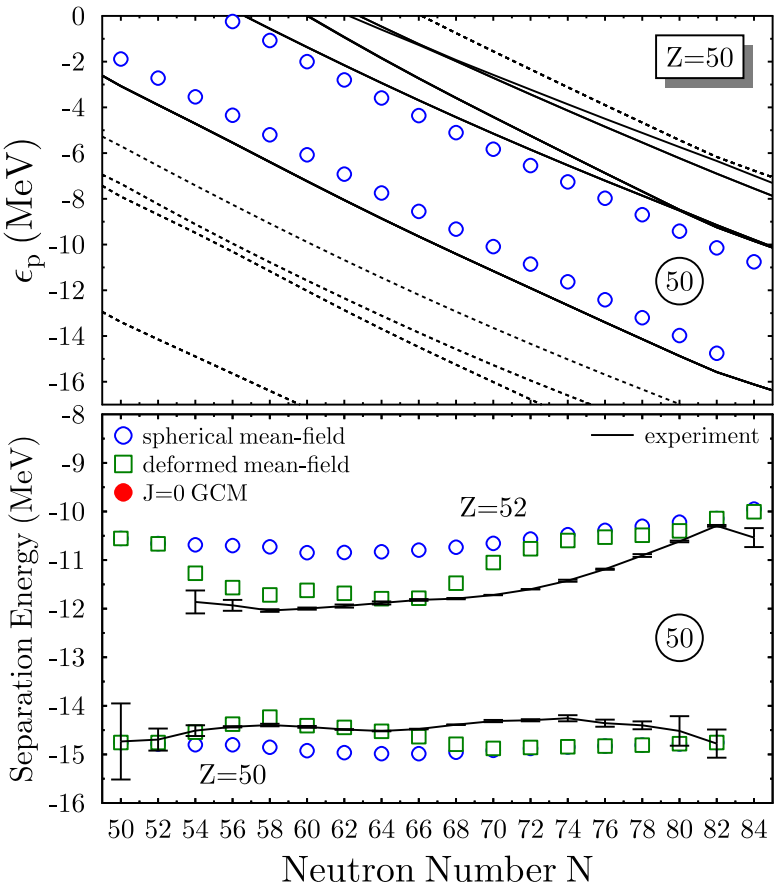
M. B., G. F. Bertsch, P.-H. Heenen, PRC 78 (2008) 054312

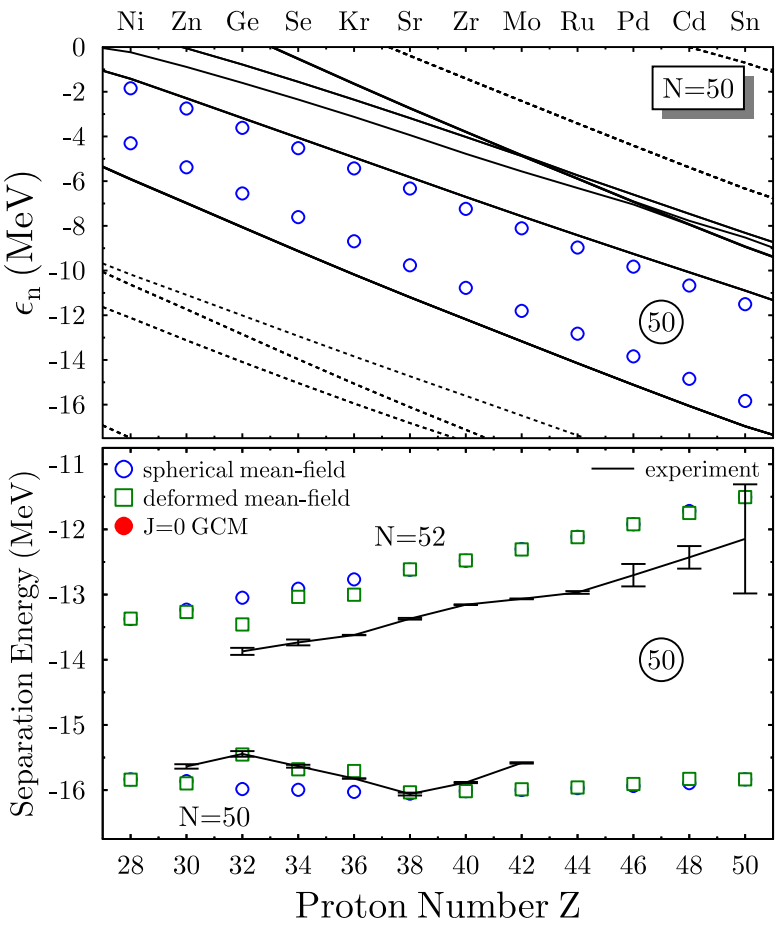
lower panel: $-S_{2n}(Z, N=50)/2$
The global linear trend is taken out subtracting

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

using the spherical mean-field S_{2n}

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





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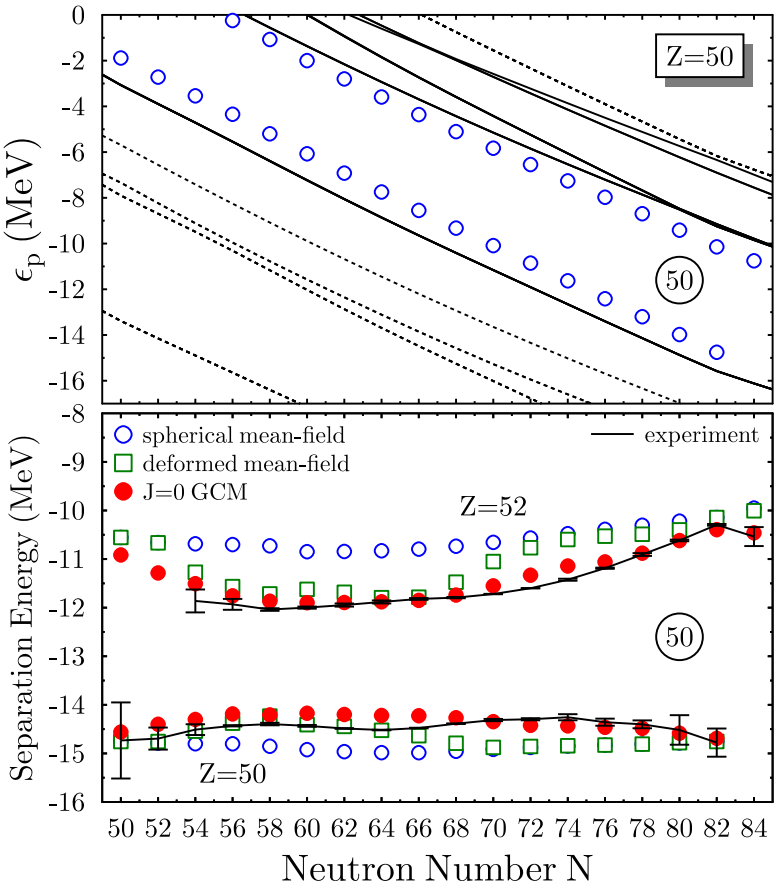

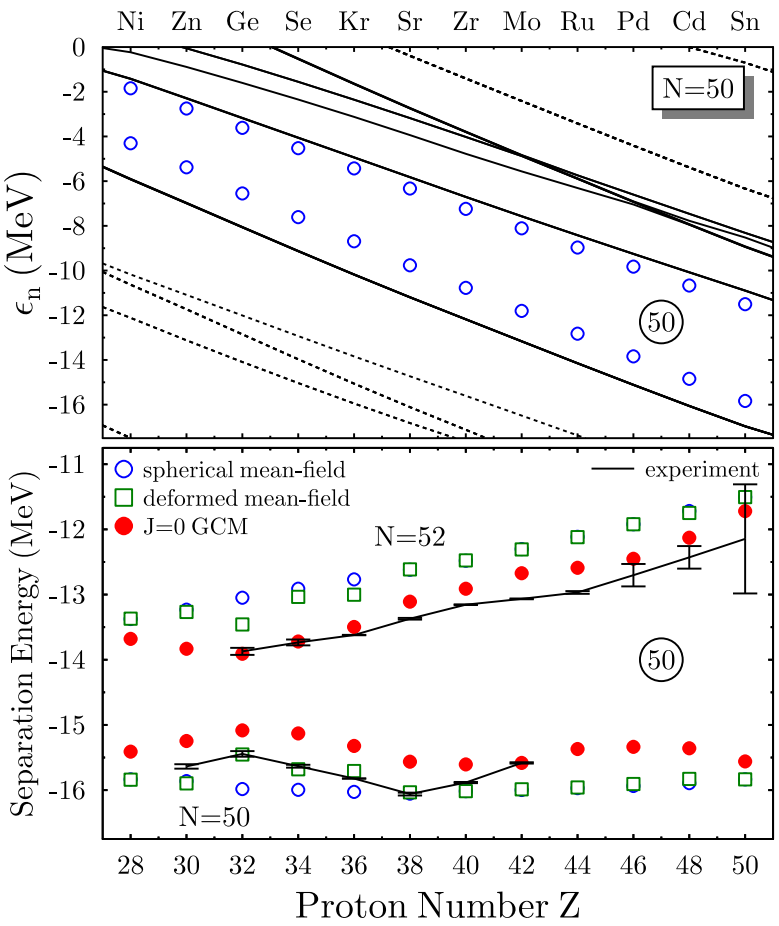

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using the spherical mean-field S_{2p}

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

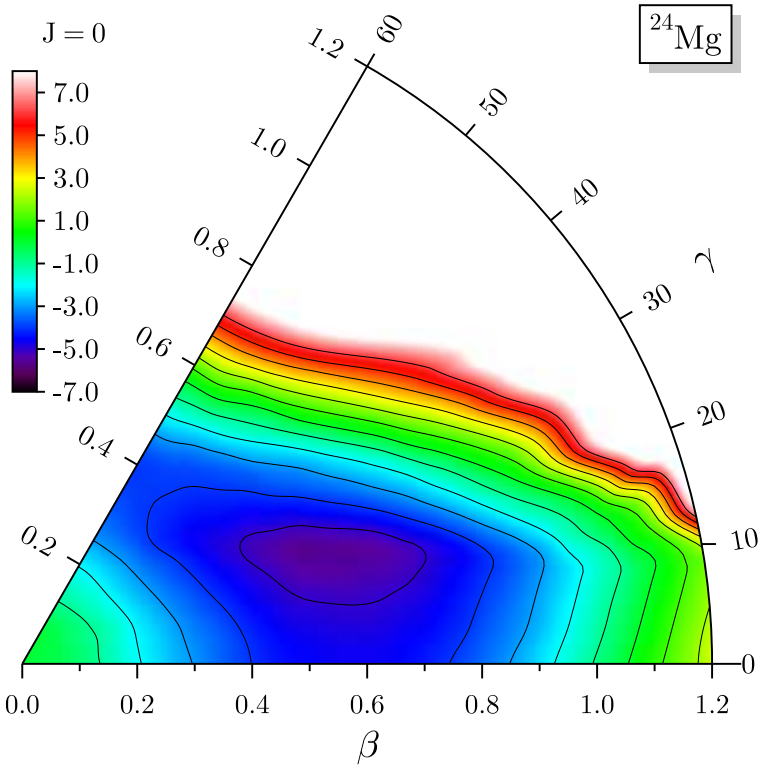
lower panel: $-S_{2n}(Z, N=50)/2$
The global linear trend is taken out subtracting

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

using the spherical mean-field S_{2n}

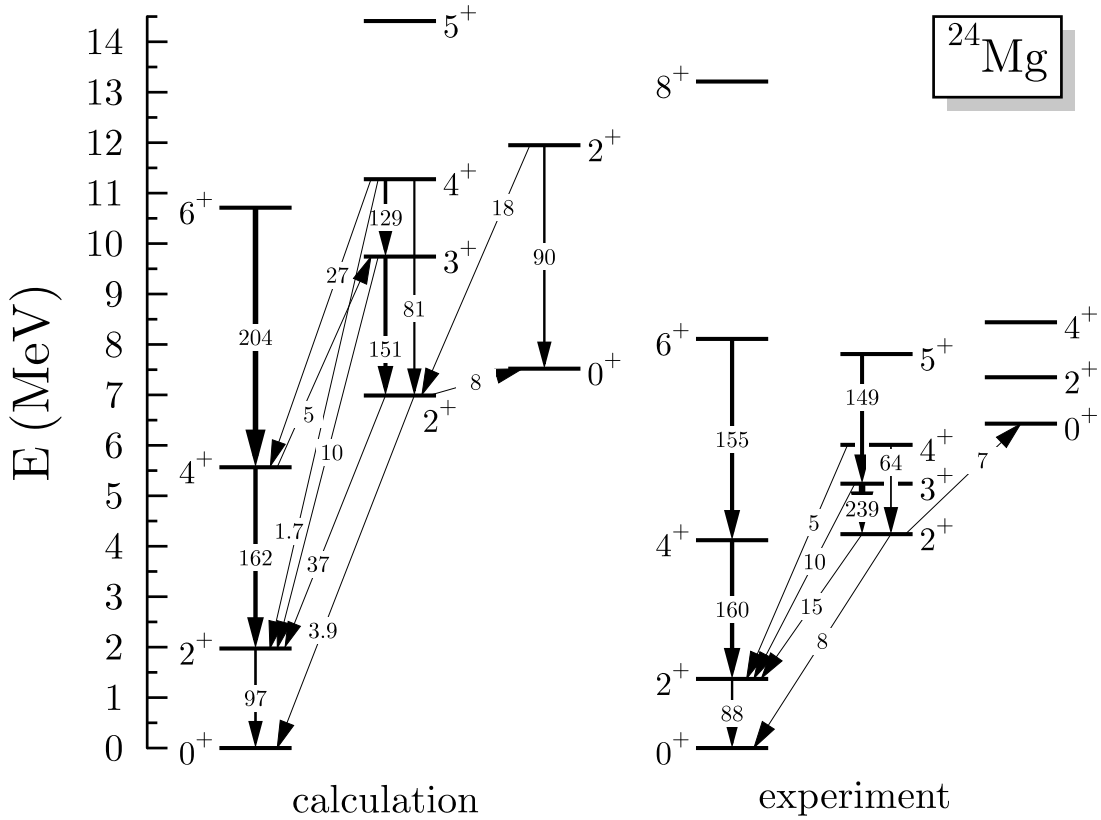
Milestones: Angular momentum projection of triaxial states

$J = 0$ projected deformation energy surface



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

excitation spectrum

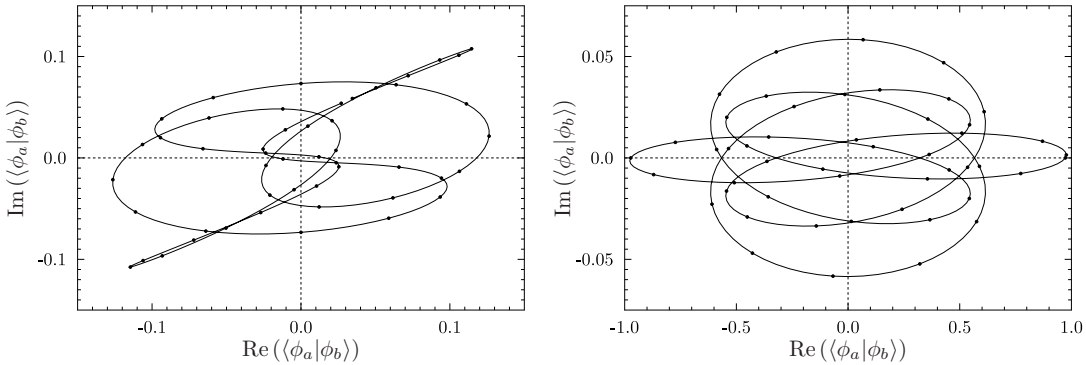


Solving the sign problem in MR EDF

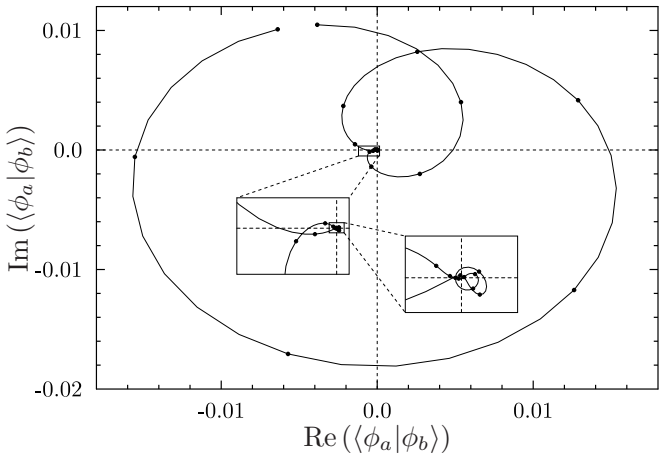
Overlap from Pfaffian formula, Benoît Avez & M. B., PRC 85 (2012) 034255

α, β held fixed at some values, γ varied

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



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



Starting point was work by Robledo, PRC 79 (2009) 021302; Robledo, PRC 84 (2011) 014307. Similar expressions derived in Bertsch & Robledo, PRL108 (2012) 042505.

New developments: use angular-momentum optimized states

Limitations of the existing implementations of the method

- limited to even-even nuclei
- collective states only
- excitation spectra too spread out

What is the missing physics?

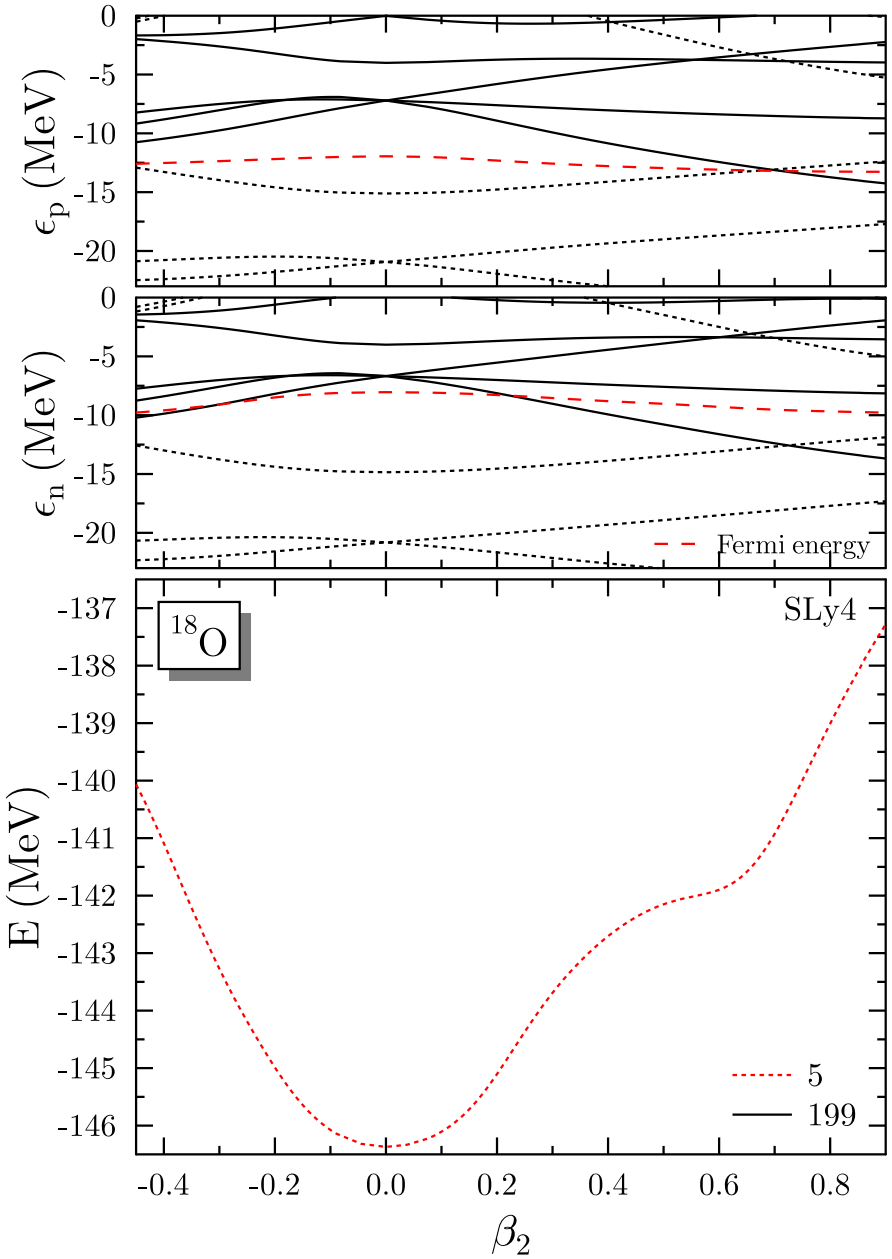
- explicit coupling to single-particle degrees of freedom

How to introduce the missing physics?

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

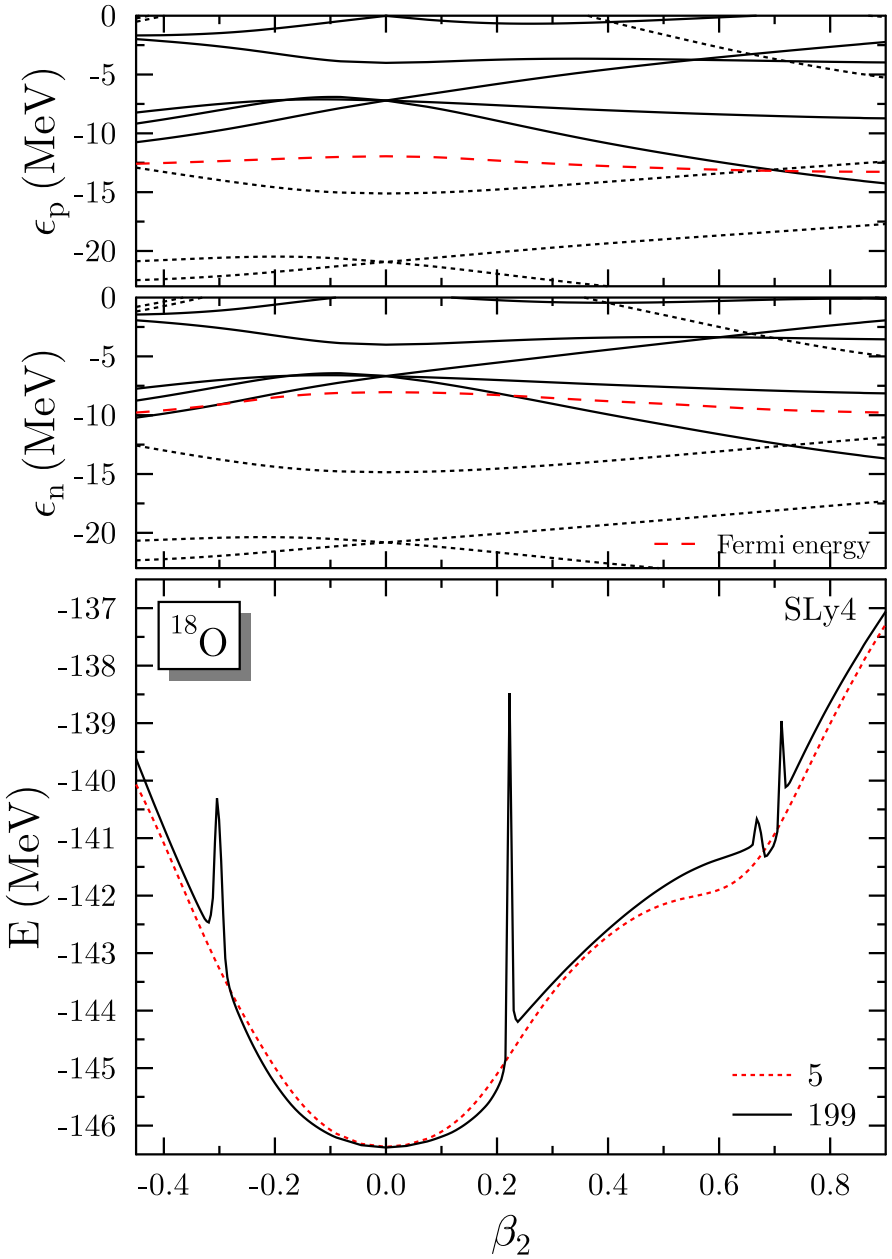
+ adjustment of improved energy functionals

Problems . . .



- pure particle-number projection

Problems . . .



- pure particle-number projection
- first hints: Dönau, PRC 58 (1998) 872; Almehed, Frauendorf, Dönau, PRC 63 (2001) 044311; Anguiano, Egido, Robledo NPA696 (2001) 467
- First analysis in a strict energy density functional framework and of EDF-specific consequences by Dobaczewski, Stoitsov, Nazarewicz, Reinhard, PRC 76 (2007) 054315
- 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, Duguet, Heenen, Lacroix, *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 under particle exchange when calculating the energy, leading to non-physical interactions of a given nucleon or pair of nucleons with itself
- these self-interactions remain (usually) hidden in the mean field
- in the extension to symmetry-restored GCM, these terms cause
  - discontinuities and divergences in symmetry-restored energy surfaces
  - breaking of sum rules in symmetry restoration
  - potentially multi-valued EDF in case of standard density-dependencies

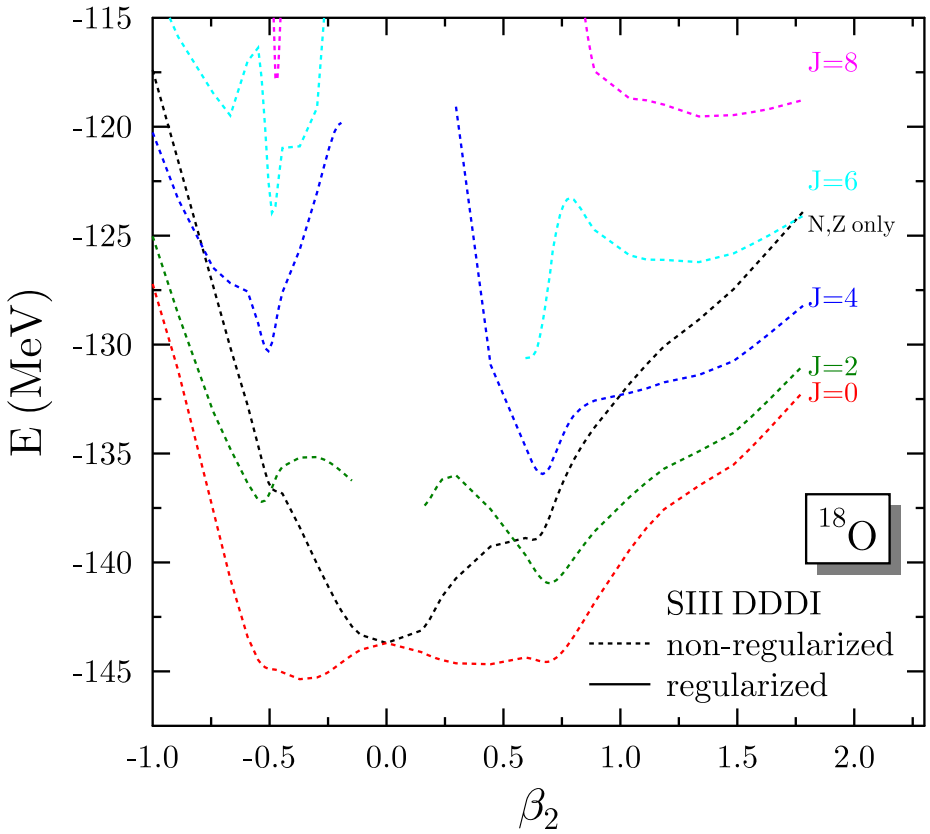
What to do?

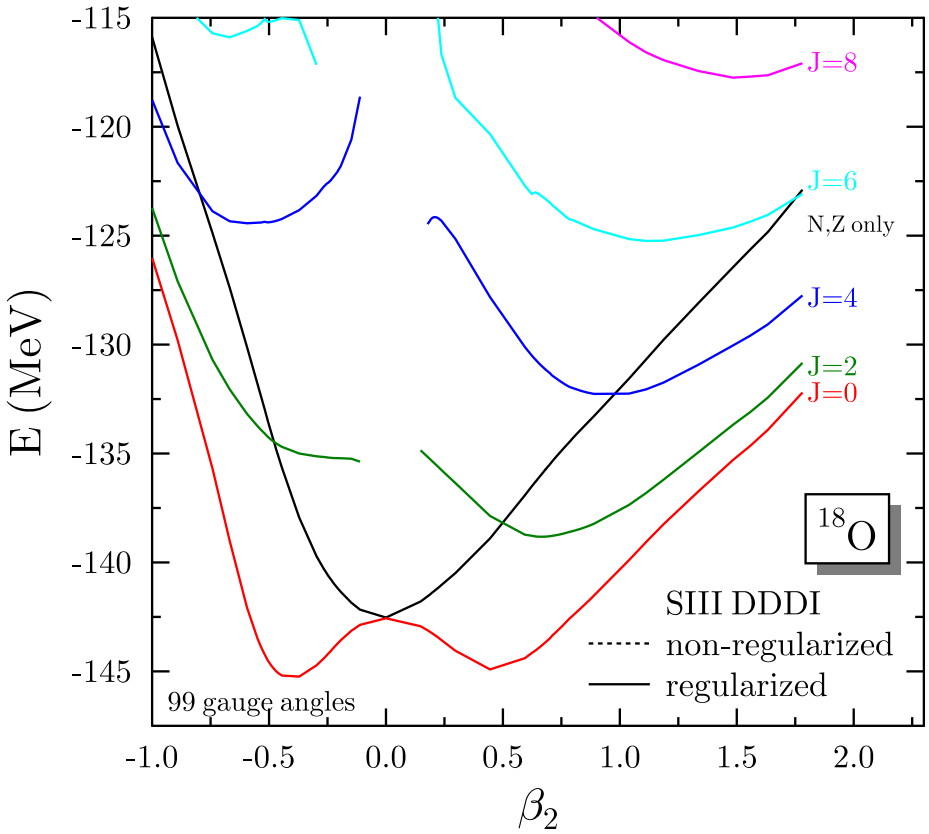
1. constructing the EDF as expectation value of a strict Hamiltonian. New problem: numerically very costly due to Coulomb exchange & pairing; no available parameterizations of high quality (the difficulties to construct such parametrizations was the main motivation to use EDFs in the 1970s).
2. construct the EDF from a density-dependent Hamiltonians with special treatment of the density entering density dependent terms for which numerically efficient high-quality parameterizations can be easily constructed. Problem: numerically very costly due to Coulomb exchange & pairing; cannot be defined for all possible confifuration mixing [Robledo, J. Phys. G 37 (2010) 064020].
3. introducing a regularization scheme of the EDF that allows for the use of (almost) standard functionals [Lacroix, Duguet, & Bender, PRC 79 (2009) 044318] for which numerically efficient high-quality parameterizations can be easily constructed [Washiyama, Bennaceur, Avez, Bender, Heenen, & Hellemans, PRC 86 (2012) 054309]. Problem: complicated formalism.

We tried the last option first.

The regularisation: it *almost* works

Usual number of Euler and gauge angles:

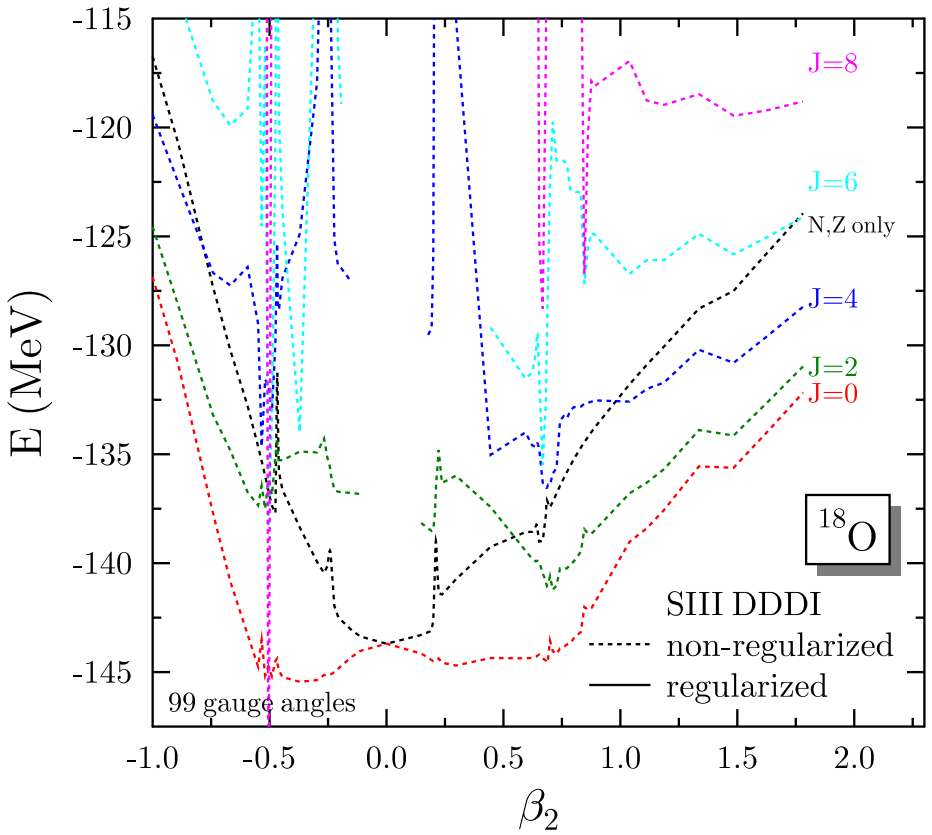


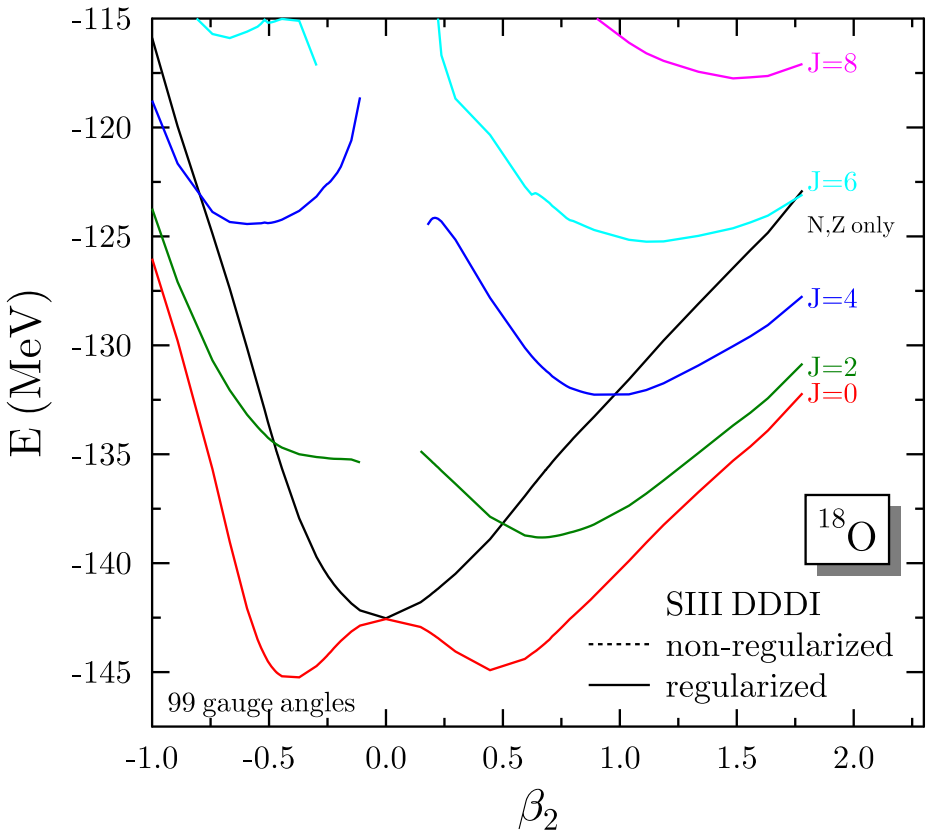


M. B., B. Avez, T. Duguet, P.-H. Heenen, D. Lacroix, unpublished

The regularisation: it *almost* works

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

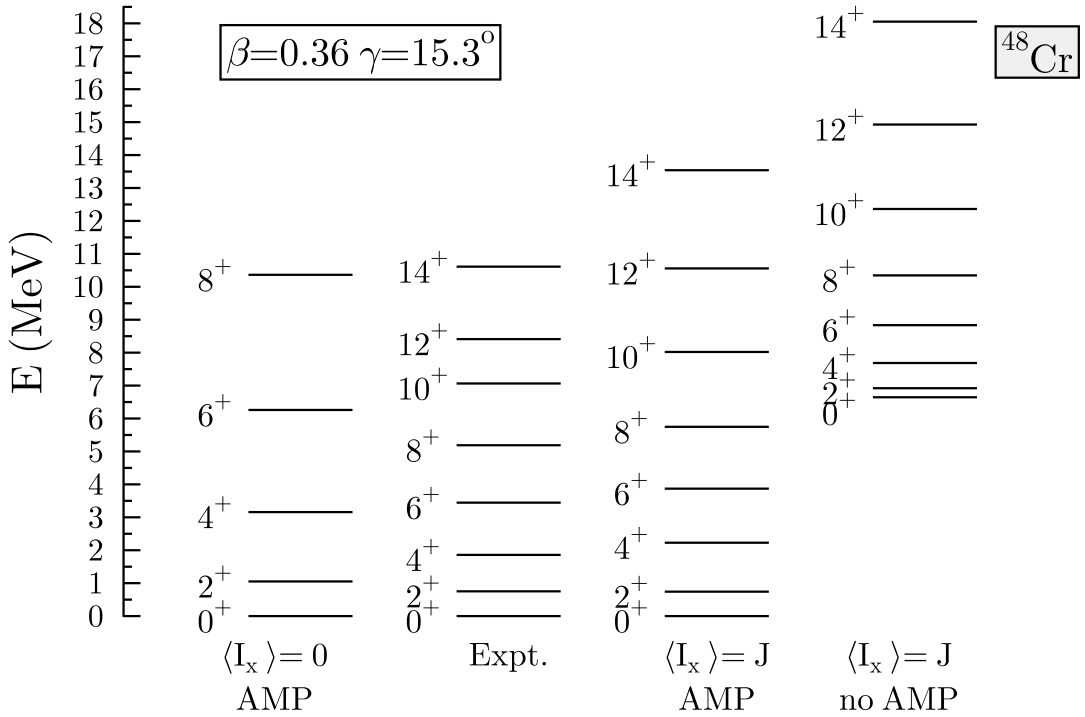




M. B., B. Avez, T. Duguet, P.-H. Heenen, D. Lacroix, unpublished

$\Rightarrow$ dependence on the discretization that becomes visible only when using unreasonably fine discretizations

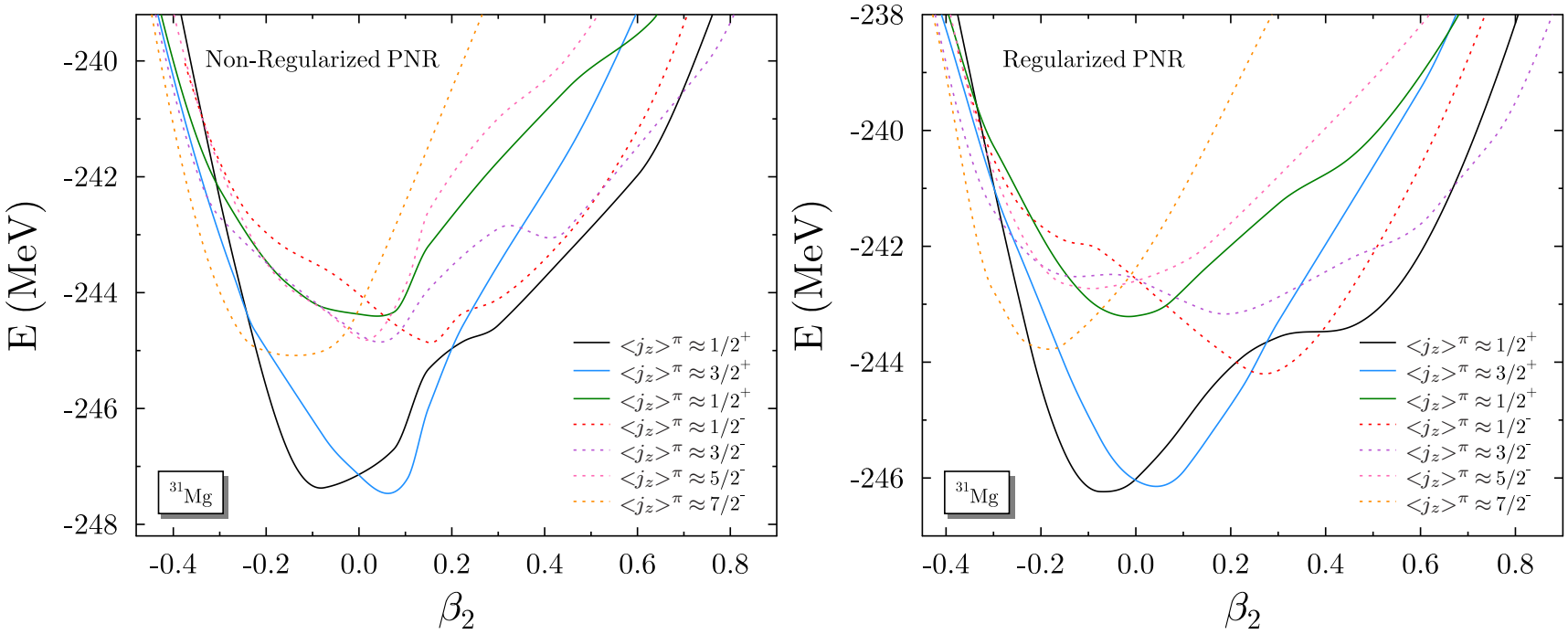
Projecting cranked HFB states



- spectra projected from cranked states are (almost) realistic only when regularising
- improved moment of inertia at low spin
- reproduction of backbending requires scanning the whole energy surface

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

Particle-number restoration of ^{31}Mg

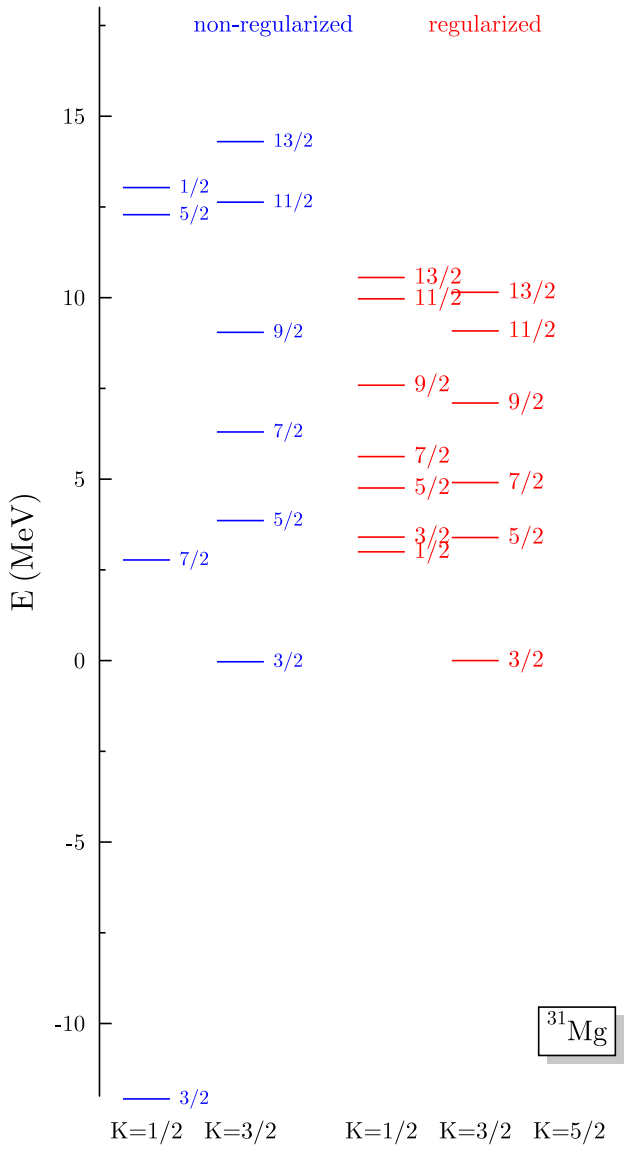


B. Bally, B. Avez, M. B., P.-H. Heenen (unpublished)

All states are constructed as blocked one-quasiparticle HFB states

The regularization can become large

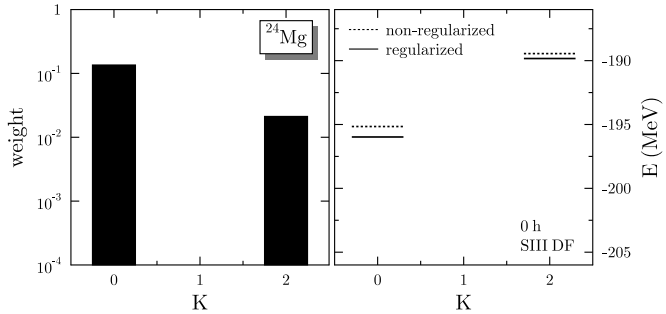
J	K	weight	E_{nonreg}	regul	E_{reg}
1	1	0.001006	−234.071	10.037	−244.108
3	1	0.001809	−259.183	−15.481	−243.702
5	1	0.001820	−234.818	7.531	−242.349
7	1	0.001797	−244.332	−2.848	−241.484
9	1	0.001271	−267.849	−28.332	−239.517
11	1	0.000902	−201.965	35.172	−237.137
13	1	0.000544	−336.901	−100.352	−236.549
3	3	0.039376	−247.137	−0.032	−247.105
5	3	0.030730	−243.247	0.467	−243.714
7	3	0.023390	−240.805	1.395	−242.199
9	3	0.013372	−238.060	1.948	−240.007
11	3	0.007914	−234.473	3.548	−238.021
13	3	0.004087	−232.805	4.150	−236.956
5	5	0.000015	−582.874	−371.932	−210.942
7	5	0.000014	−103.953	94.559	−198.512
9	5	0.000010	−127.945	95.658	−223.603
11	5	0.000007	860.956	1075.711	−214.755
13	5	0.000004	−530.816	−334.758	−196.058
7	7	0.000005	790.818	977.088	−186.270
9	7	0.000004	−2215.259	−1916.331	−298.928
11	7	0.000003	−3657.395	−3321.042	−336.353
13	7	0.000002	−4077.760	−3715.879	−361.881

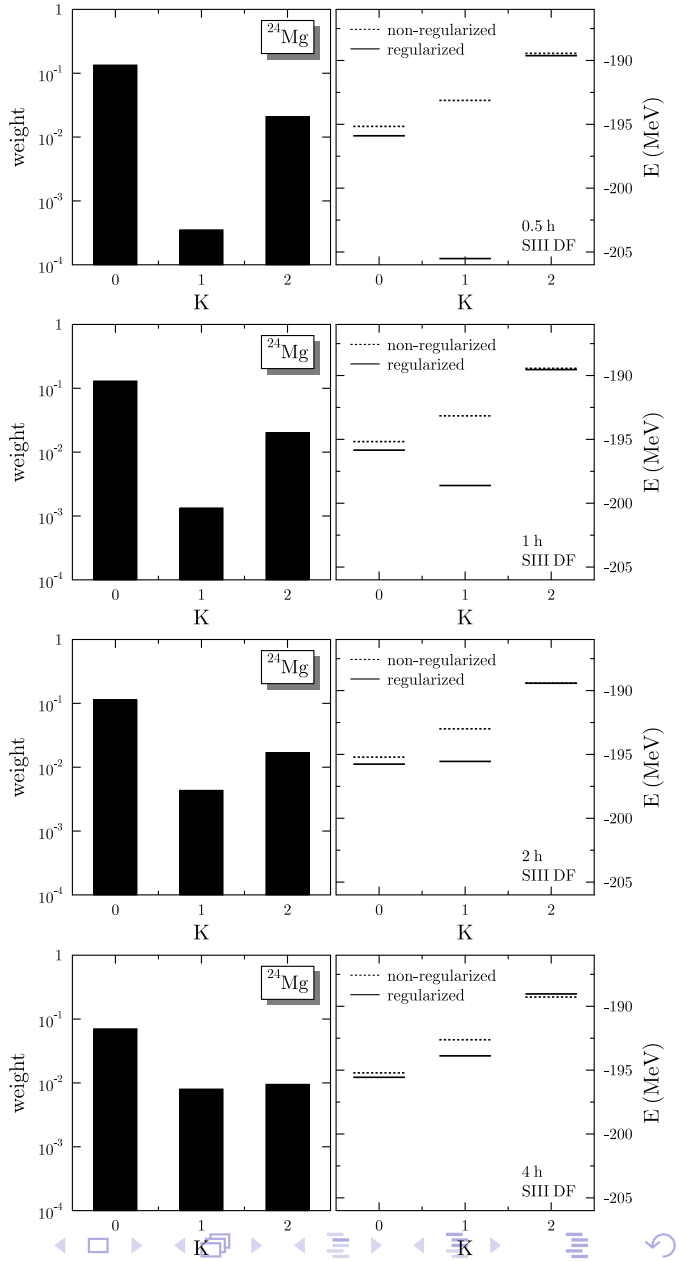


B. Bally, B. Avez, M. B., P.-H. Heenen, unpublished

There are remaining problems

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





Again: What to do?

1. constructing the EDF as expectation value of a strict Hamiltonian. New problem: numerically very costly due to Coulomb exchange & pairing; no available parameterizations of high quality (the difficulties to construct such parametrizations was the main motivation to use EDFs in the 1970s).
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3. introducing a regularization scheme of the EDF that allows for the use of (almost) standard functionals [Lacroix, Duguet, & Bender, PRC 79 (2009) 044318] for which numerically efficient high-quality parameterizations can be easily constructed [Washiyama, Bennaceur, Avez, Bender, Heenen, & Hellemans, PRC 86 (2012) 054309]. Problem: complicated formalism.

At last, we try the first option.

How to construct a suitable Hamiltonian?

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

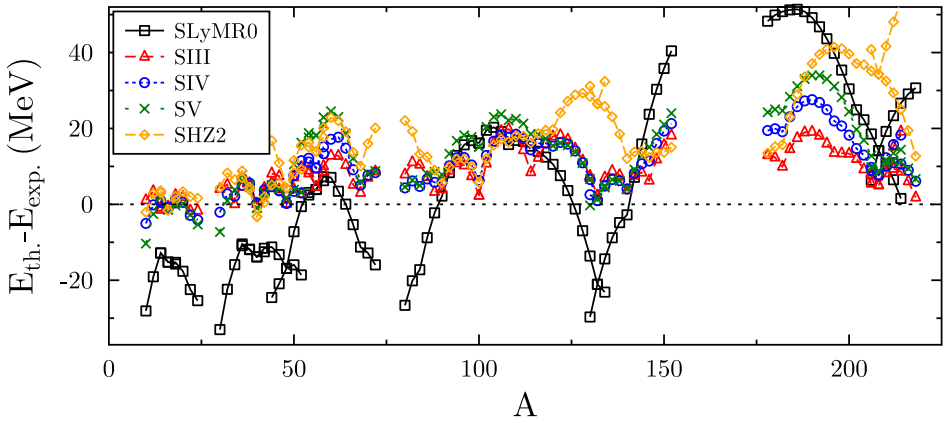
  which was the reason to introduce density dependences etc. in the 1970s.

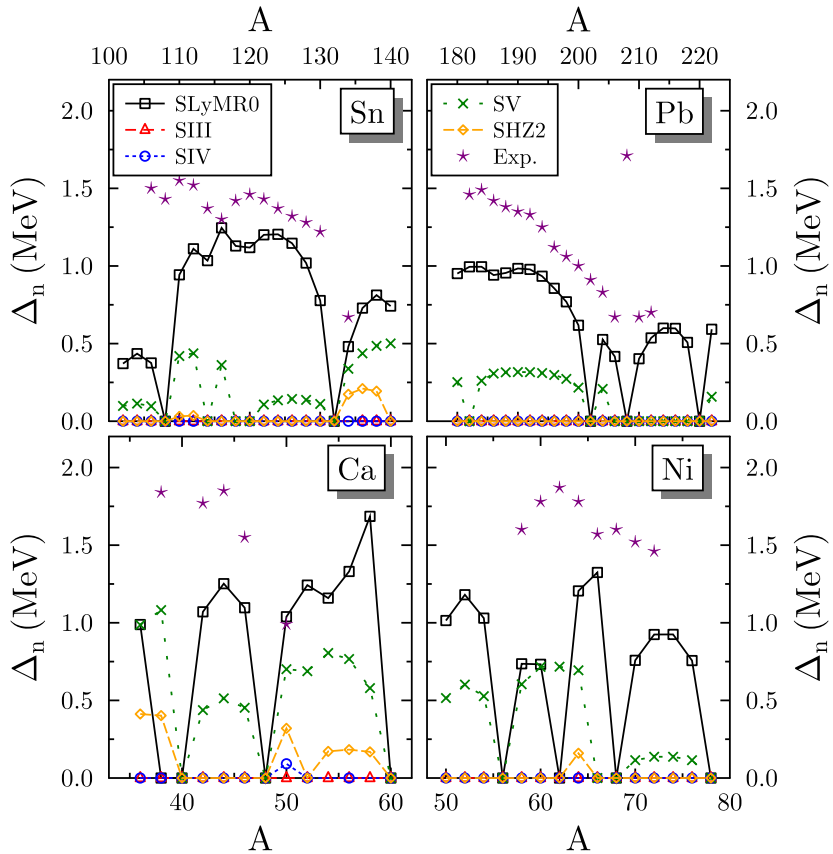
First try: SLyMR0

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

J. Sadoudi, M. Bender, K. Bennaceur, D. Davesne, R. Jodon, and T. Duguet, Physica Scripta T, *in press*

First try: standard two-body + contact 3-body + contact 4-body

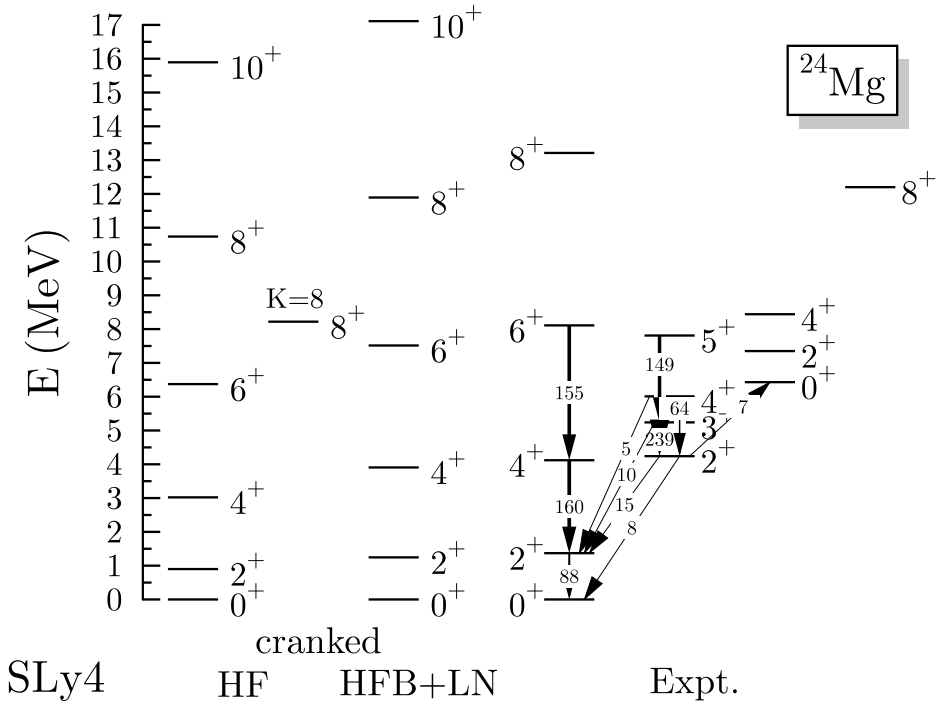




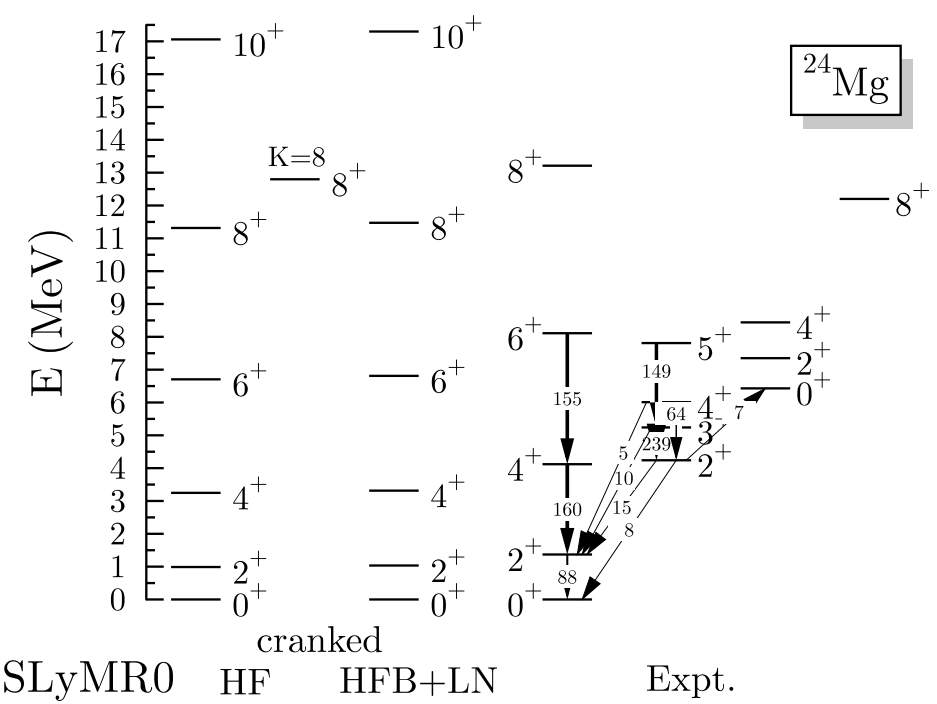
- it is impossible to fullfil the usual nuclear matter constraints , to have stable interactions and attractive pairing
- no "best fit" possible
- very bad performance compared to stanrad functionals

J. Sadoudi, M. Bender, K. Bennaceur, D. Davesne, R. Jodon, and T. Duguet, Physica Scripta, *in press*

MR EDF based on cranked HFB states: The example of ^{24}Mg



SR EDF (cranked HF & HFB+LN) using SLy4



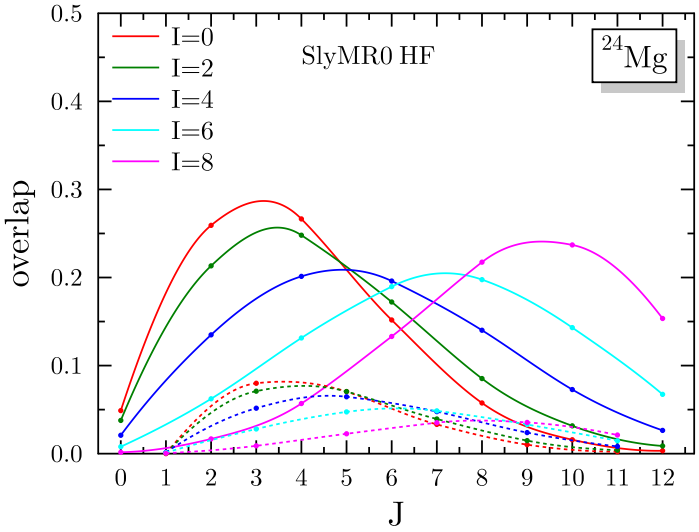
SR EDF (cranked HF & HFB+LN) using SLyMR0

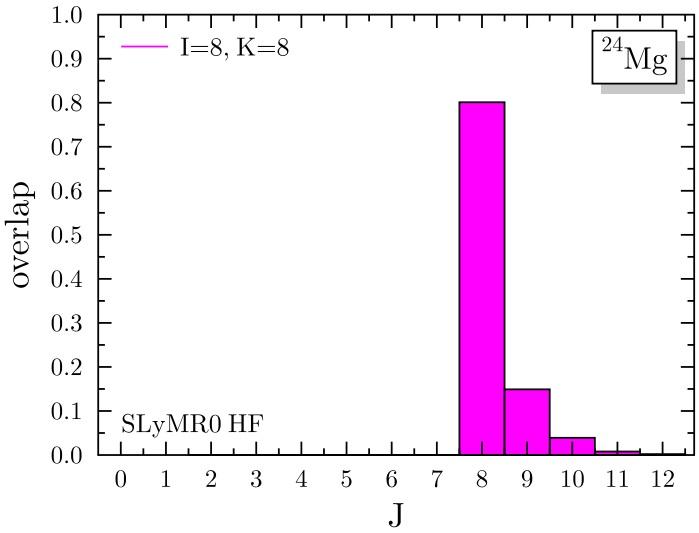
$\Rightarrow$ SLyMR0 is not completely desastrous for the description of this phenomenon

$\Rightarrow$ deformation of HF and HFB+LN is very different for SLyMR0

Decomposition of states

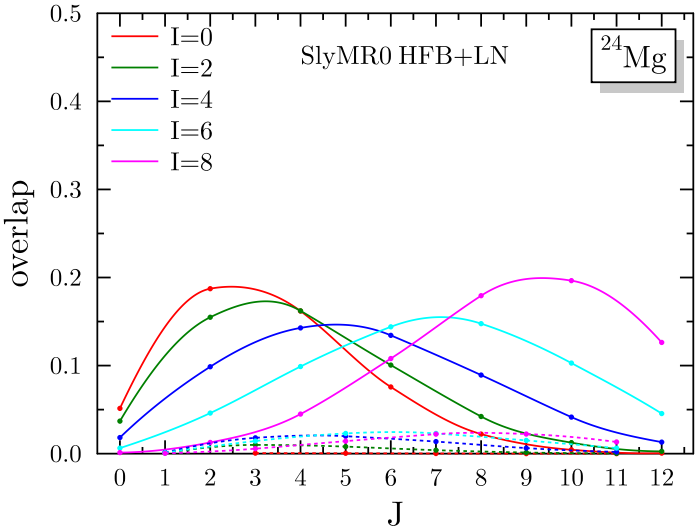
cranked HF ground state



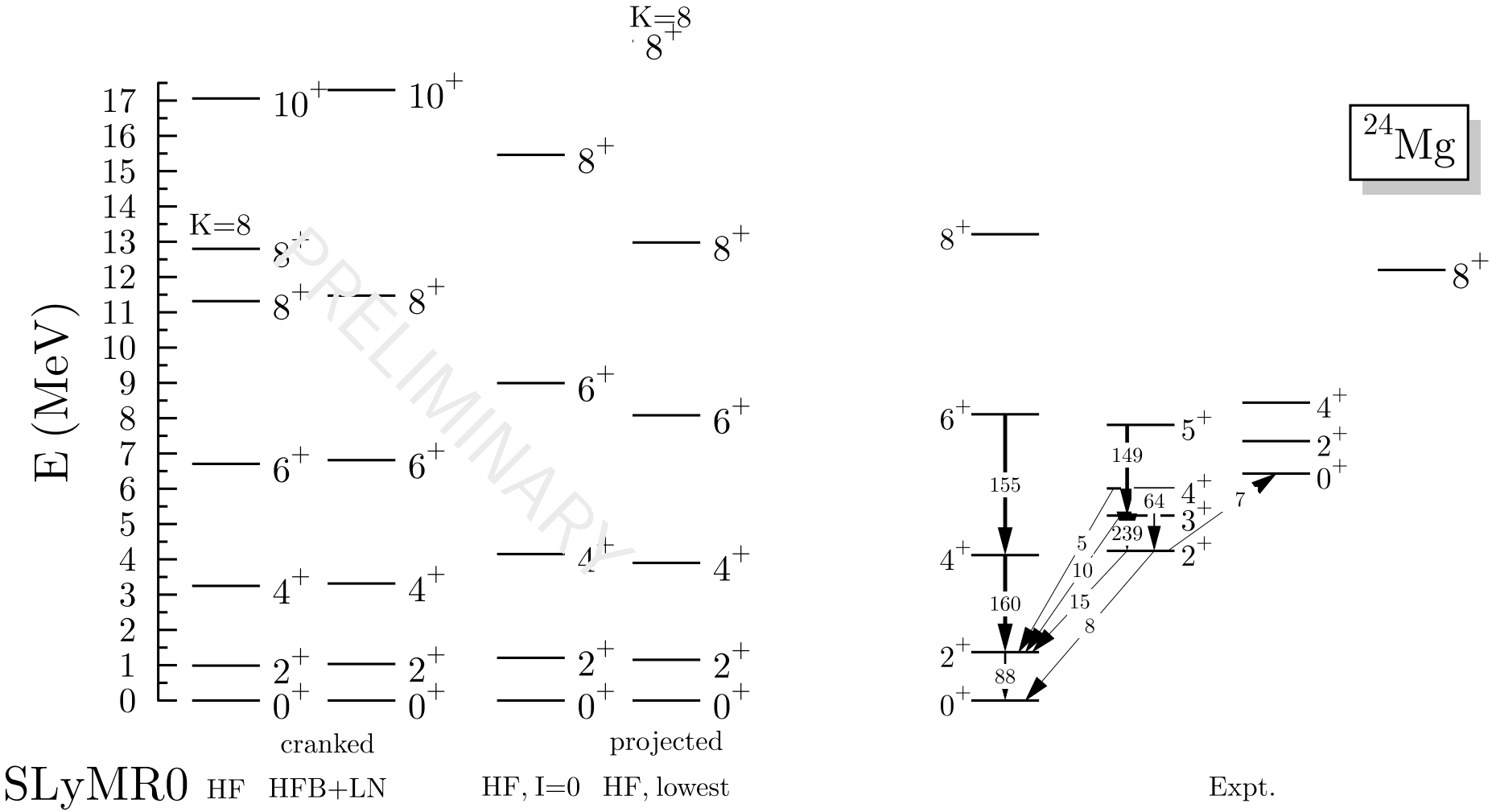


HF $K = 8$ state

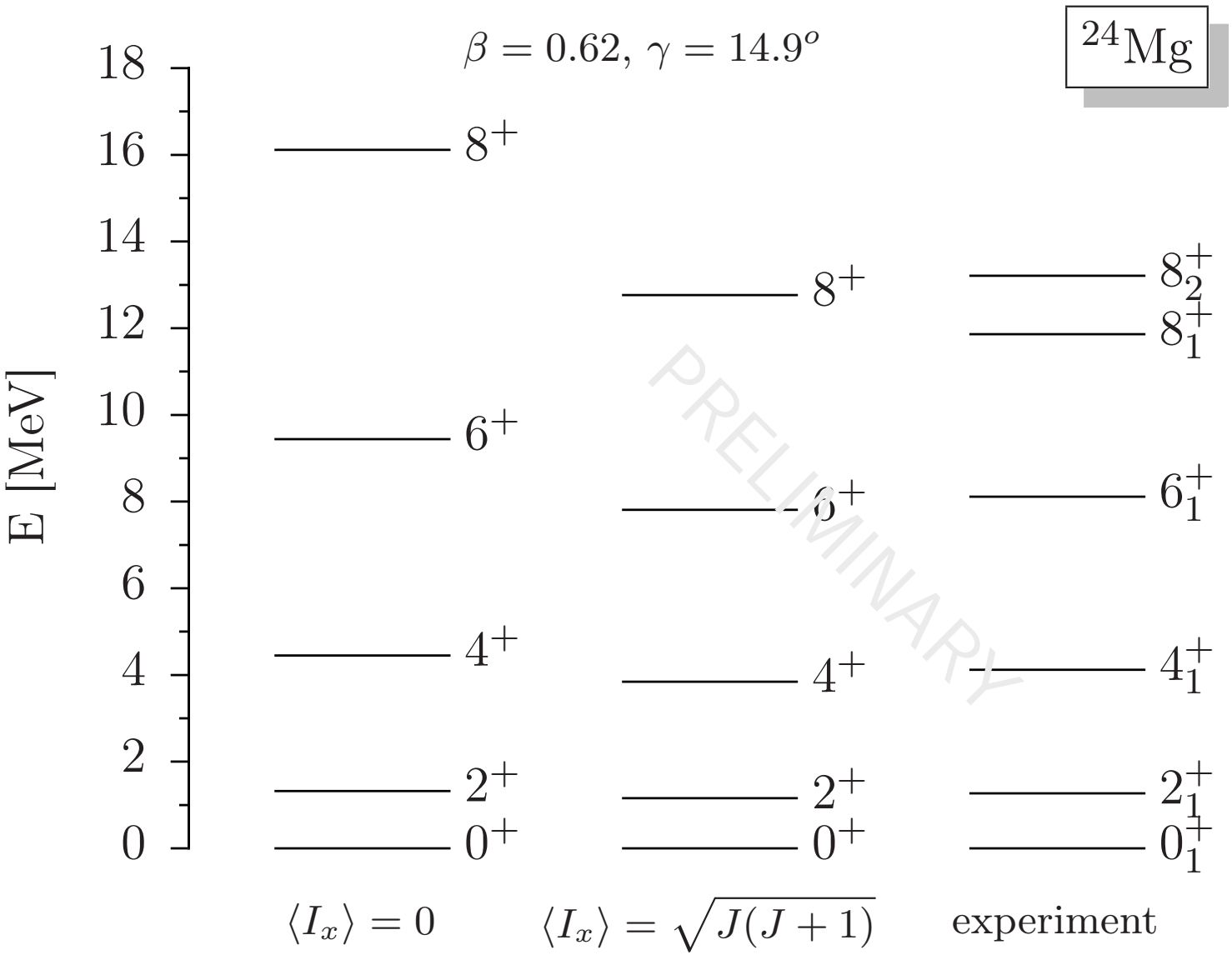
cranked HFB+LN ground state



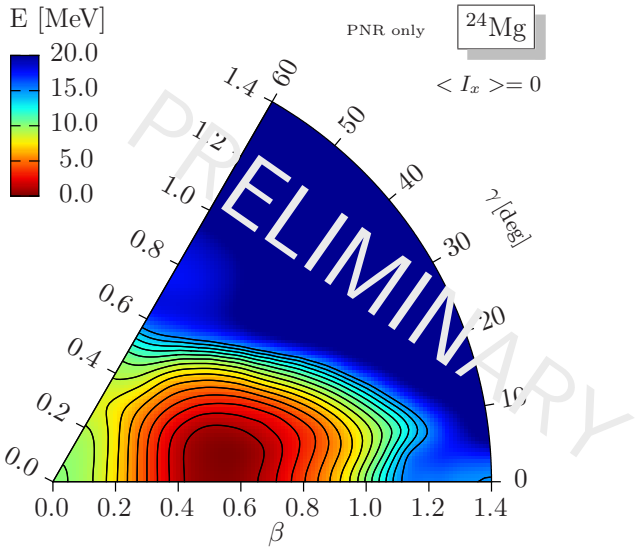
Decomposition

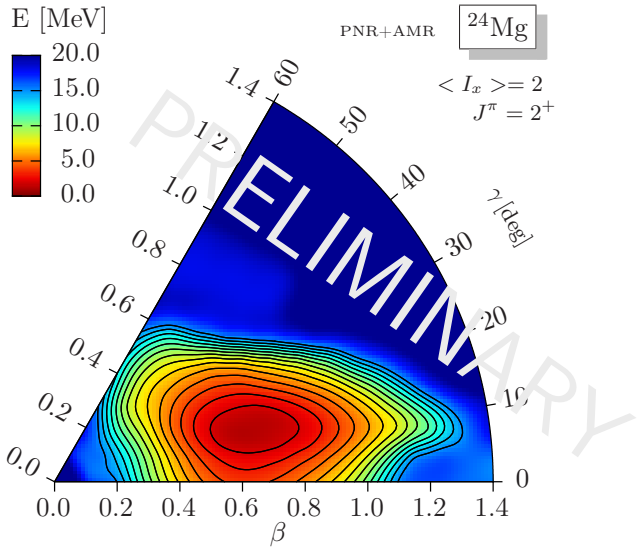


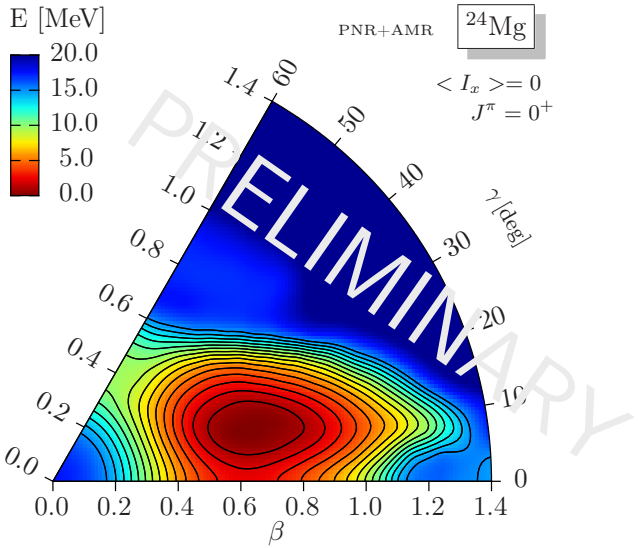
Decomposition



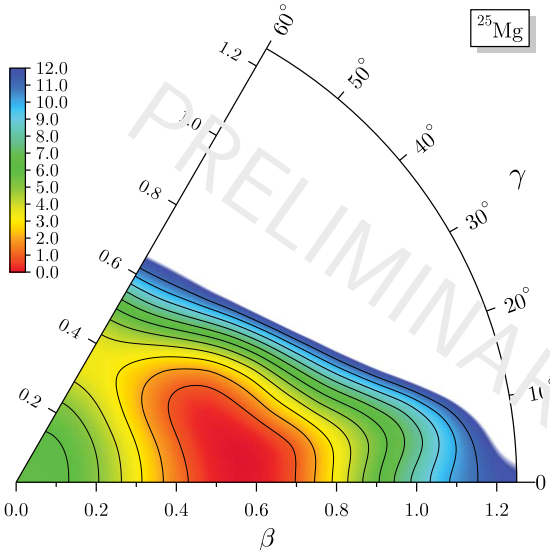
Energy surfaces





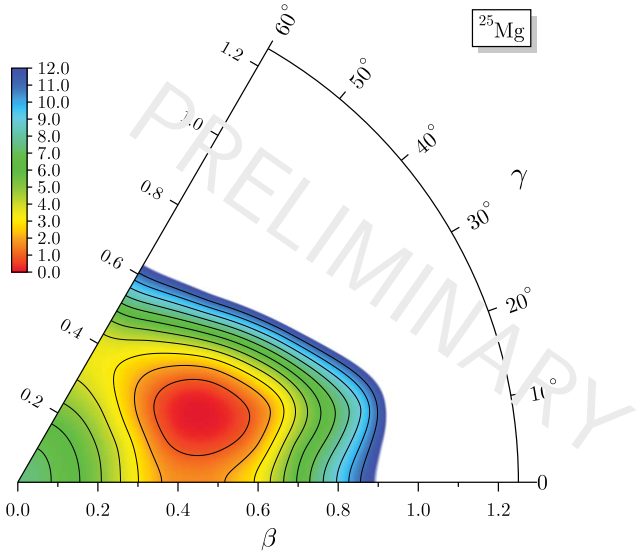


Odd-A nuclei with SLyMR0: The example of ^{25}Mg

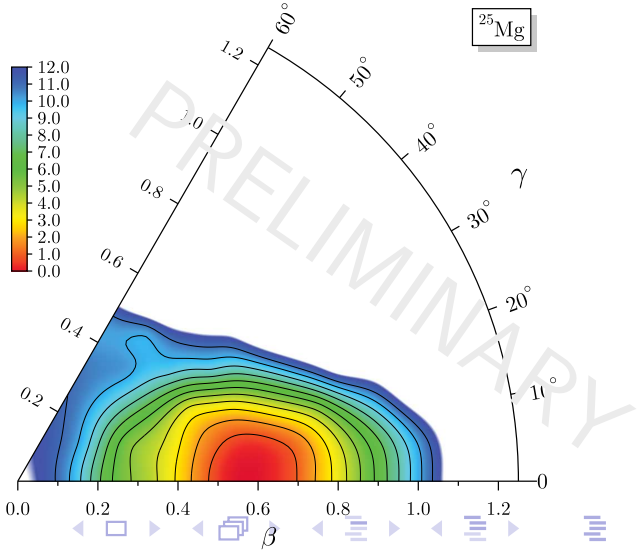


"False vacuum" (non-blocked HFB ground state with $\langle \hat{N} \rangle = 13$, $\langle \hat{Z} \rangle = 12$)

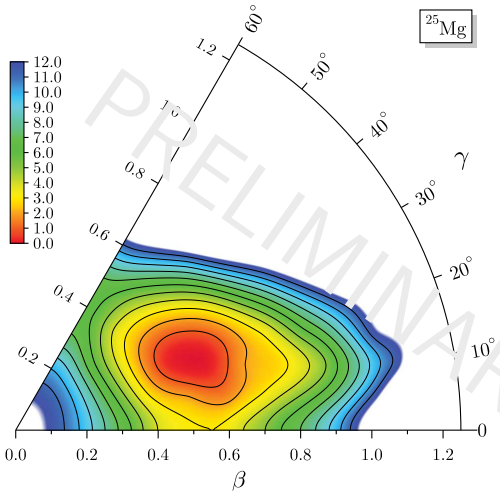
B. Bally, B. Avez, M. B., P.-H. Heenen (to be published)



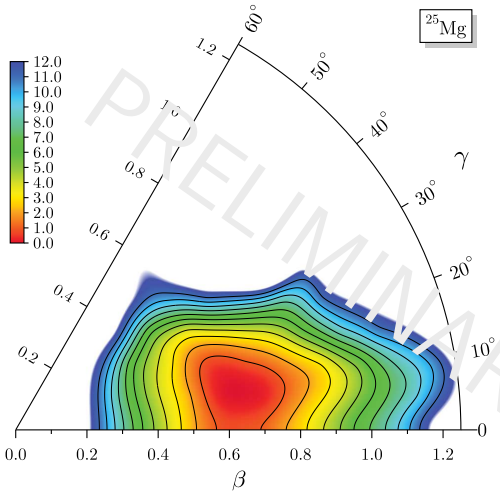
Blocked HFB 1-quasiparticle state, where blocked particle has $\langle j_z \rangle \approx 5/2$



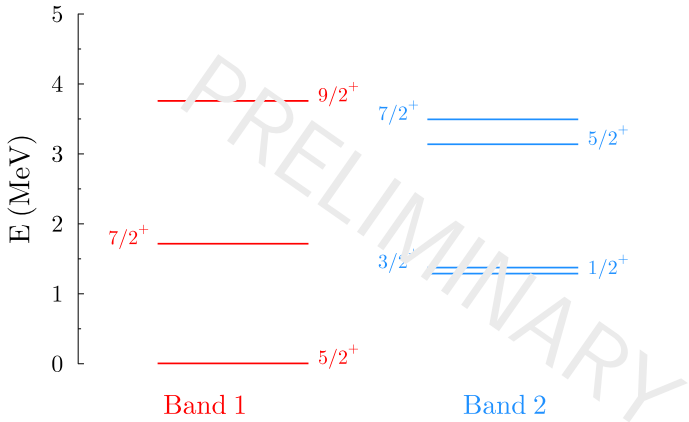
First "beyond-mean-field" results for odd-A nuclei with SLyMR0



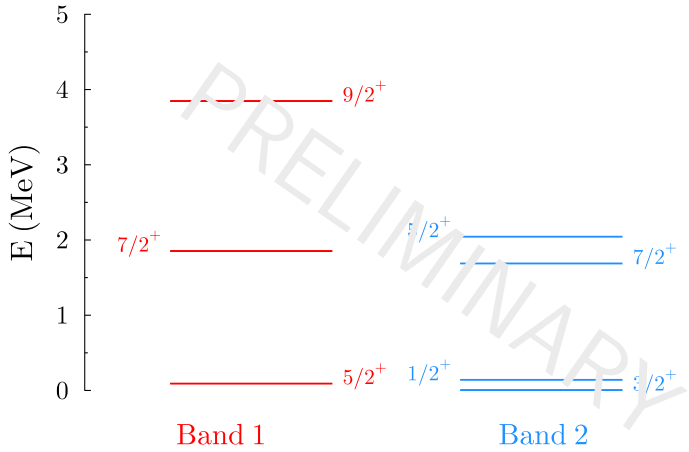
Blocked 1-qp state with $\langle j_z \rangle \approx 5/2$, projected on $Z = 12$, $N = 13$, $J = 5/2^+$.



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



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



Full GCM of projected states.

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

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

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

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

Take-away messages

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

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

Publications are in preparation.