Symmetry-restored GCM with EDFs: new developments, problems, perspectives

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What to expect from this presentation

- For the story so far, please refer to the presentation by Paul-Henri Heenen.
- Distinguish "exact" GCM solving the Hill-Wheeler-Griffin equation from solving an *m*d collective Bohr-type Hamiltonian derived via GOA
- "Exact" symmetry restoration and exact GCM allow to benchmark approximate schemes used to describe fission dynamics (error bars)
- (Exact) GCM is *not* only a theory for collective motion, but also describes
  - coupling of single-particle degrees of freedom and collective degrees of freedom
  - the collective motion of excited quantum-mechanical states
- using *time-reversal invariance breaking HFB states* (*n*-quasiparticle blocking, constraint on $\langle \hat{J}_i \rangle$, ...) extends the range of applicability and the predictive power of symmetry-restored GCM
- exact GCM can only be done in a controlled way with *Hamiltonians* **without** density dependences and **without** making approximations and/or generalizations, which requires a new class of *pseudo-potential-generated EDFs* as opposed to the currently used *general EDFs*.

Commercial break

Long-term goals of our project:

- 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.

GCM based on "angular-momentum optimized" states

Limitations of the existing *implementations* of the method as (implicitely) outlined in the talk by Paul-Henri Heenen

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

What is the missing physics?

- explicit coupling of single-particle degrees of freedom to collective motion

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 n-quasiparticle HFB states describe single-particle excitations (non-adiabatic states in general, K isomers, odd-A nuclei, odd-odd nuclei)

+ adjustment of improved energy functionals

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

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 $\mathbf{q}$

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

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

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

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

with

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

Angular-momentum projected GCM gives the

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

Necessary developments

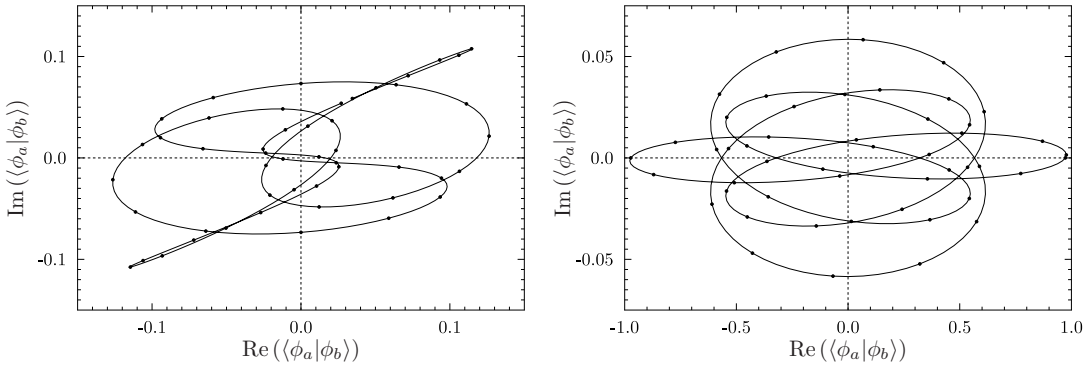
- technical: solve sign problem in Onishi's formula for the overlap!
- conceptual: what kind of functionals to use?
- practical: how to construct the model space of N-body states?

Solving the sign problem in MR EDF

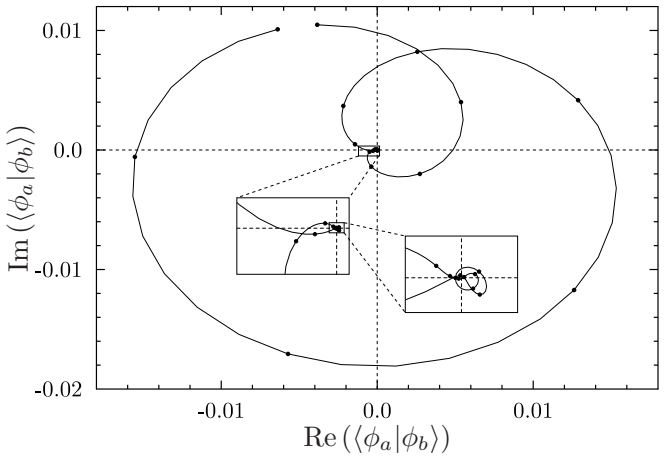
Overlap from Pfaffian formula, Benoît Avez & M. B., PRC 85 (2012) 034255

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.

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

$$E_{\mathbf{q}}^{HFB} = \langle \mathrm{SR}_{\mathbf{q}} | \hat{H} | \mathrm{SR}_{\mathbf{q}} \rangle$$

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

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

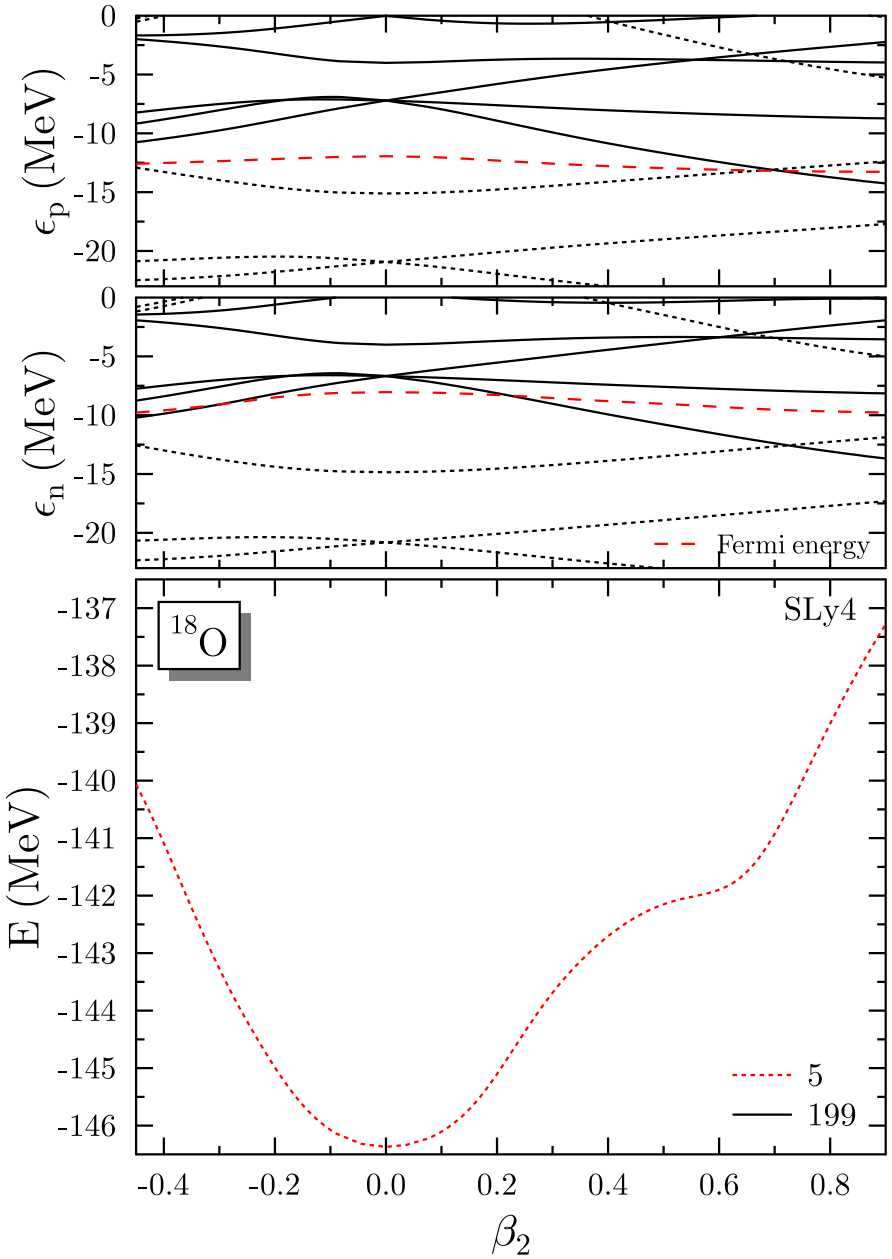
- GCM: coherent superposition of Slater determinants/HFB states

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

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

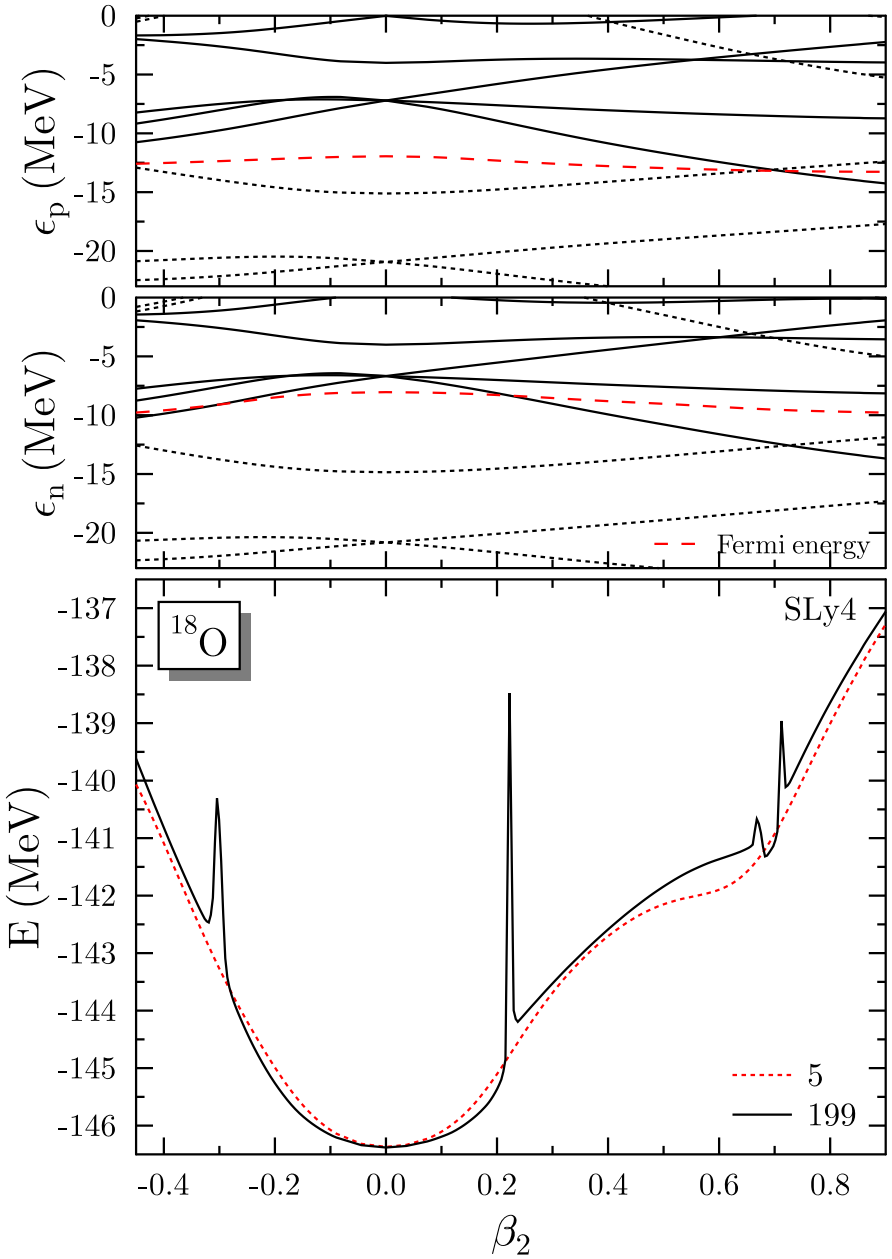
$$\mathcal{E}_\mu^{\mathrm{MR}} = \sum_{q,q'} f_\mu^*(\mathbf{q}) \, \mathcal{E}_{\mathbf{qq}'}^{\mathrm{MR}}[\rho_{\mathbf{qq}'}, \kappa_{\mathbf{qq}'}, \kappa_{\mathbf{qq}'}^*] \, f_\mu(\mathbf{q}') \quad \text{where} \quad \rho_{\mathbf{qq}'} = \langle \mathrm{SR}_{\mathbf{q}} | \hat{\rho} | \mathrm{SR}_{\mathbf{q}'}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

What kind of functionals to use? Problems with existing ones



- pure particle-number projection

What kind of functionals to use? Problems with existing ones



- pure particle-number projection
- first hints from Hamiltonian-based approaches: 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 (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, 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 ("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-dependencies

Functionals corresponding to "true Hamiltonians" vs. "true" functionals

True contact pseudo-potential $t_0\,(1+x_0\hat{P}_\sigma)\,\delta(\mathbf{r}-\mathbf{r}')$

$$\begin{aligned}\mathcal{E} &= \int d^3r\,\Big\{\tfrac{3}{8}\,t_0\,\rho_0^2(\mathbf{r}) - \tfrac{1}{8}\,t_0\,(1+2x_0)\,\rho_1^2(\mathbf{r}) - \tfrac{1}{8}\,t_0\,(1-2x_0)\,\mathbf{s}_0^2(\mathbf{r}) \\ &\quad -\tfrac{1}{8}\,t_0\,\mathbf{s}_1^2(\mathbf{r}) + \tfrac{1}{8}\,t_0\,(1+x_0)\,\check{\mathbf{s}}_0(\mathbf{r})\cdot\check{\mathbf{s}}_0^*(\mathbf{r}) + \tfrac{1}{8}\,t_0\,(1-x_0)\,\check{\rho}_1(\mathbf{r})\,\check{\rho}_1^*(\mathbf{r})\Big\}\end{aligned}$$

(see Perlinska *et al.* PRC 69 (2004) 014316 for definition of $\check{\mathbf{s}}_0(\mathbf{r})$ and $\check{\rho}_1(\mathbf{r})$)

Contact functional:

$$\begin{aligned}\mathcal{E} &= \int d^3r\,\Big\{C_0^\rho[\rho_0,\ldots]\,\rho_0^2(\mathbf{r}) + C_1^\rho[\rho_0,\ldots]\,\rho_1^2(\mathbf{r}) + C_0^s[\rho_0,\ldots]\,\mathbf{s}_0^2(\mathbf{r}) \\ &\quad + C_1^s[\rho_0,\ldots]\,\mathbf{s}_1^2(\mathbf{r}) + C_0^{\check{s}}[\rho_0,\ldots]\,\check{\mathbf{s}}_0(\mathbf{r})\cdot\check{\mathbf{s}}_0^*(\mathbf{r}) + C_1^{\check{\rho}}[\rho_0,\ldots]\,\check{\rho}_1(\mathbf{r})\,\check{\rho}_1^*(\mathbf{r})\Big\}\end{aligned}$$

Coulomb interaction $\frac{e^2}{|\mathbf{r}-\mathbf{r}'|}$

$$\mathcal{E} = \frac{1}{2}\iint d^3r\,d^3r'\,\frac{e^2}{|\mathbf{r}-\mathbf{r}'|}\Big[\rho_p(\mathbf{r})\rho_p(\mathbf{r}') - \rho_p(\mathbf{r},\mathbf{r}')\rho_p(\mathbf{r}',\mathbf{r}) + \kappa_p^*(\mathbf{r},\mathbf{r}')\kappa_p(\mathbf{r},\mathbf{r}')\Big]$$

Approximate Coulomb functionals

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

Forgotten constraints in general functionals

Hamiltonian

$$\hat{H} = \sum_{ij} a_i^\dagger \, t_{ij}^{(1)} \, a_j + \frac{1}{2!} \sum_{ijkl} a_i^\dagger \, a_j^\dagger \, v_{ijkl}^{(2)} \, a_l \, a_k + \frac{1}{3!} \sum_{ijklmn} a_i^\dagger \, a_j^\dagger \, a_k^\dagger \, v_{ijklmn}^{(3)} \, a_n \, a_m \, a_l + \cdots$$

Energy

$$\begin{aligned} \langle \hat{H} \rangle &= \sum_{ij} t_{ij}^{(1)} \, \langle a_i^\dagger \, a_j \rangle + \frac{1}{2!} \sum_{ijkl} v_{ijkl}^{(2)} \, \langle a_i^\dagger \, a_j^\dagger \, a_l \, a_k \rangle + \frac{1}{3!} \sum_{ijklmn} v_{ijklmn}^{(3)} \, \langle a_i^\dagger \, a_j^\dagger \, a_k^\dagger \, a_n \, a_m \, a_l \rangle \\ &= \sum_{ij} t_{ij}^{(1)} \, \rho_{ji}^{(1)} + \frac{1}{2!} \sum_{ijkl} v_{ijkl}^{(2)} \, \rho_{lkji}^{(2)} + \frac{1}{3!} \sum_{ijklmn} v_{ijklmn}^{(3)} \, \rho_{nmlkji}^{(3)} + \cdots \end{aligned}$$

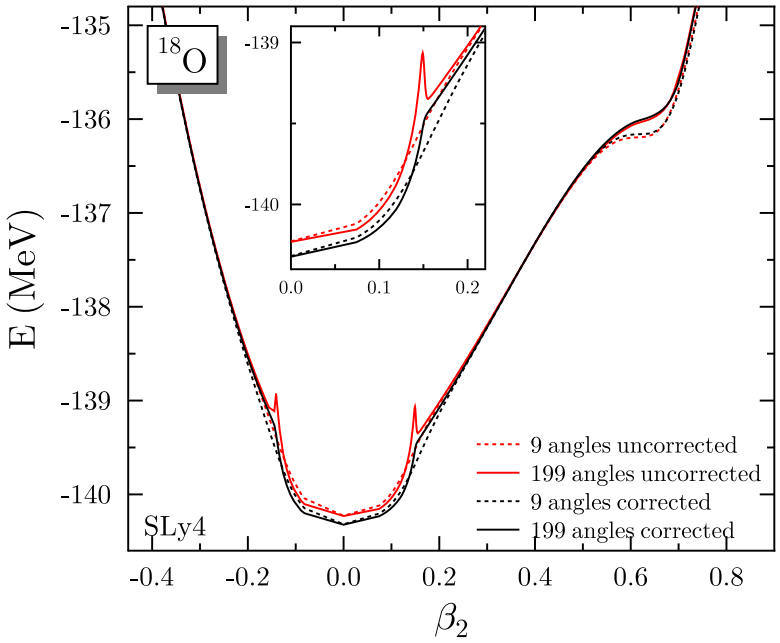
For BCS/Bogoliubov-type product states

$$\begin{aligned} \rho_{lkji}^{(2)} &= \rho_{lj}^{(1)} \, \rho_{ki}^{(1)} - \rho_{li}^{(1)} \, \rho_{kj}^{(1)} + \kappa_{ij}^{*} \, \kappa_{kl} \\ \rho_{nmlkji}^{(3)} &= \cdots \end{aligned}$$

Second problem: non-analytical density dependences

Non-viability of non-integer density dependencies

- in symmetry restored GCM, the local densities $\rho^{qq'}(\mathbf{r})$ are in general complex
- $\left[\rho^{qq'}(\mathbf{r})\right]^{\alpha}$ is a multi-valued non-analytical function
- spurious contribution from branch cuts (see 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



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

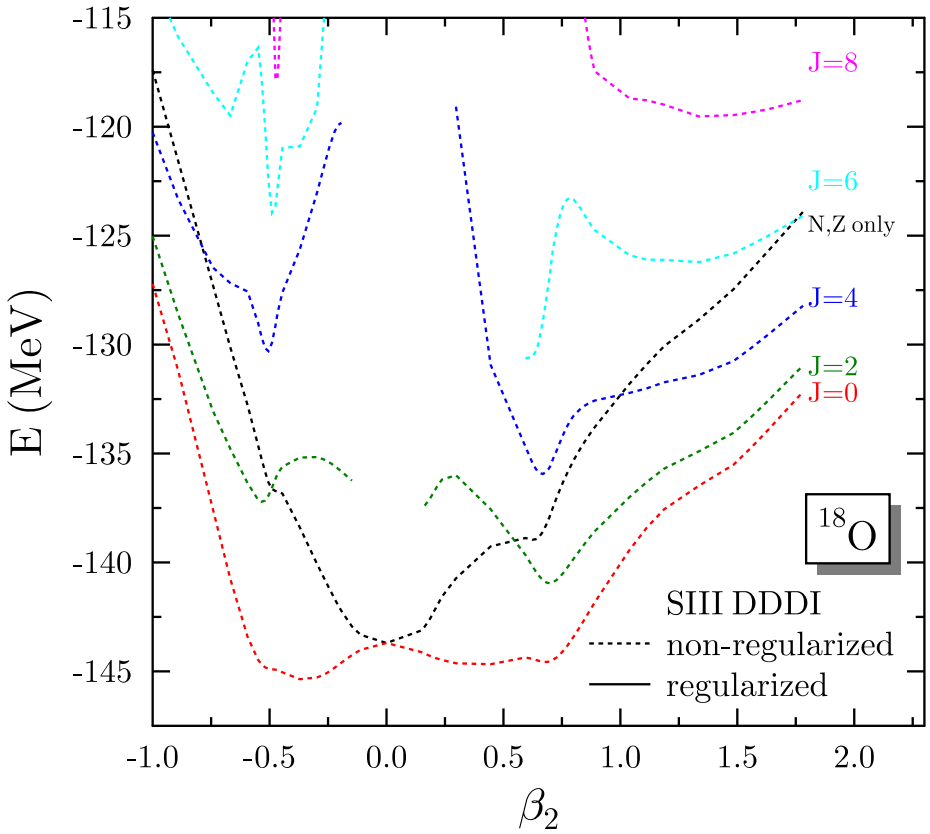
What to do?

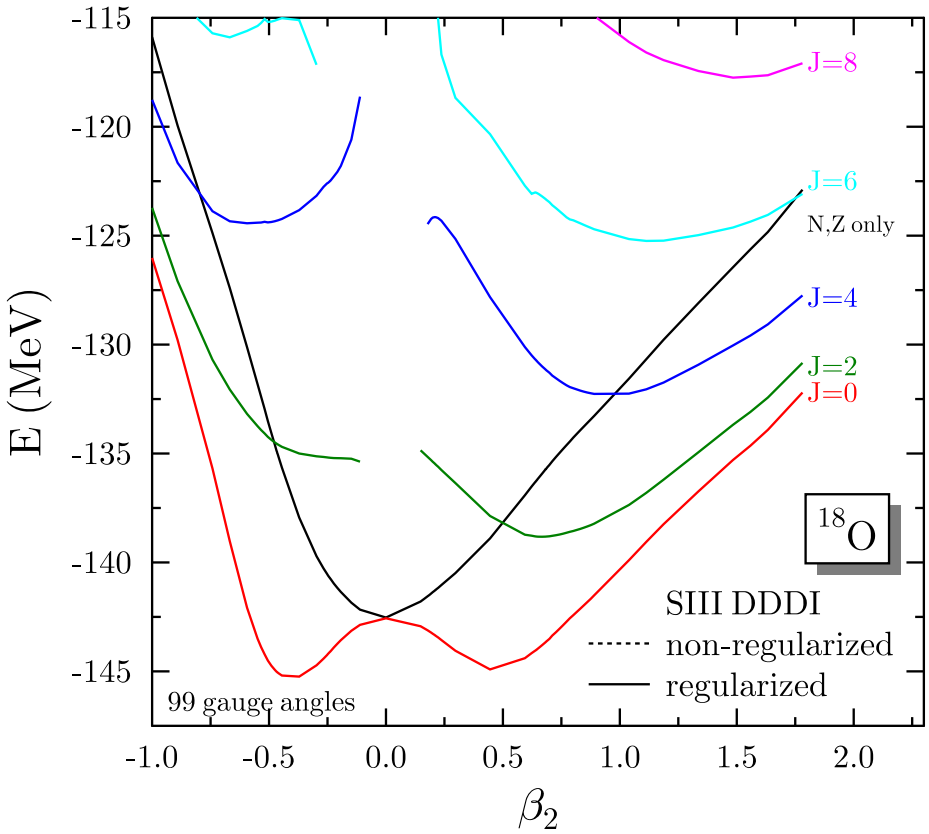
1. constructing the EDF as expectation value of a strict Hamiltonian. New problem: numerically very costly due to Coulomb exchange & pairing; no available parameterizations of high quality (the difficulties to construct such parametrizations was the main motivation to use EDFs in the 1970s).
2. construct 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:

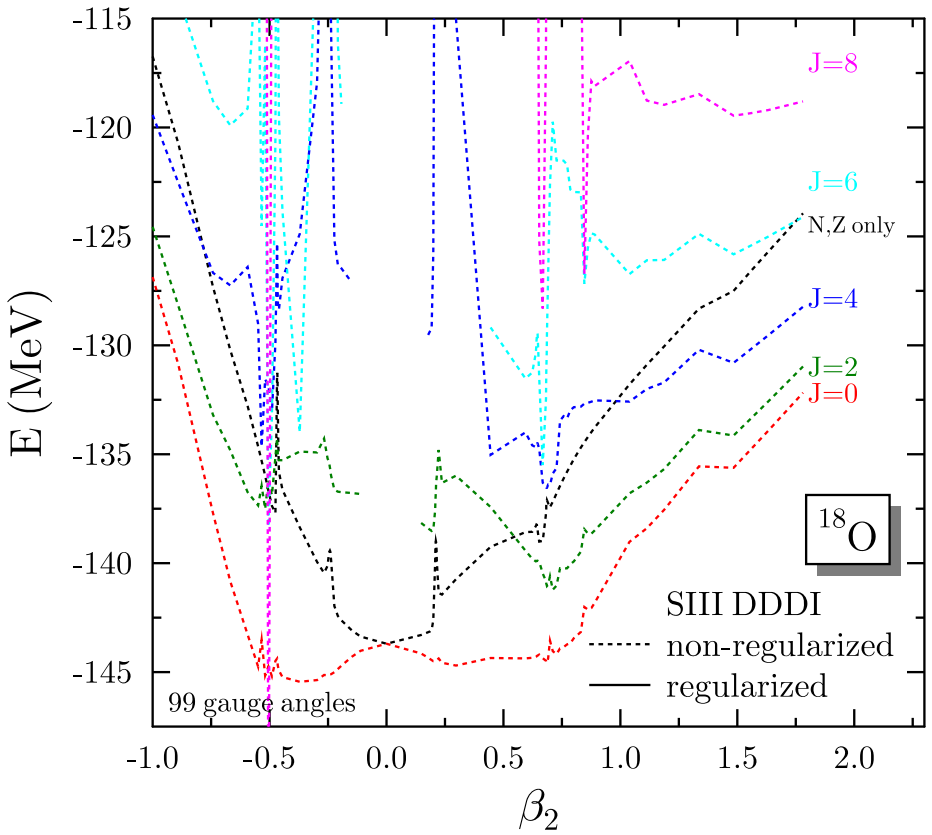


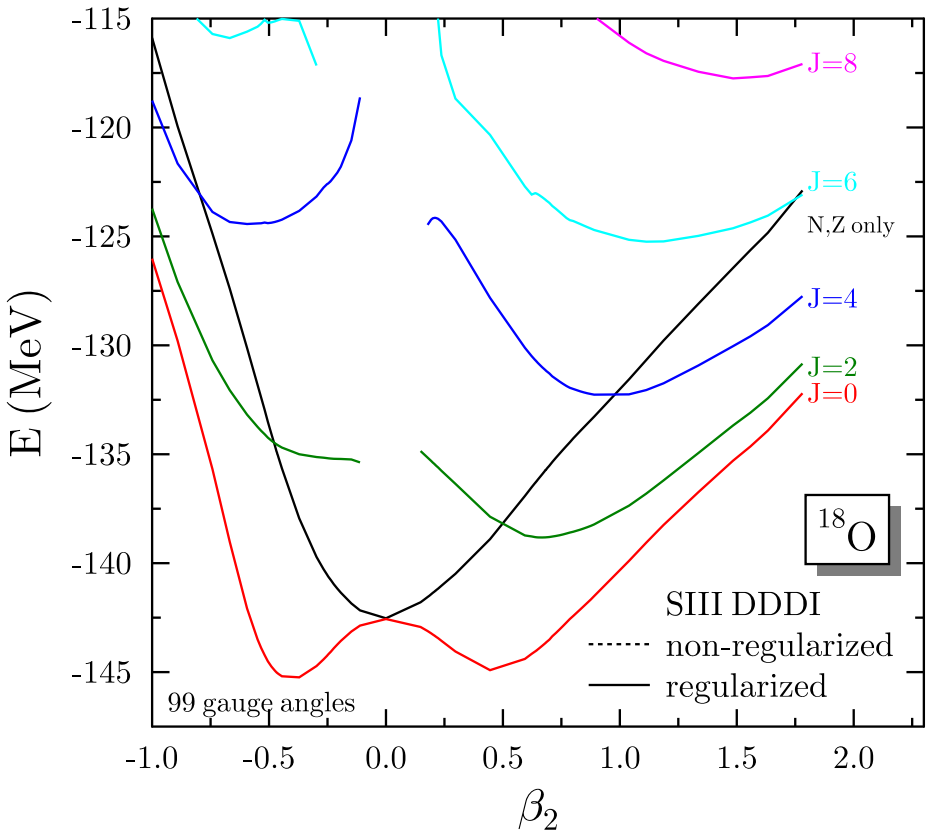


M. B., B. Avez, T. Duguet, P.-H. Heenen, D. Lacroix, unpublished

The regularisation: it *almost* works

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

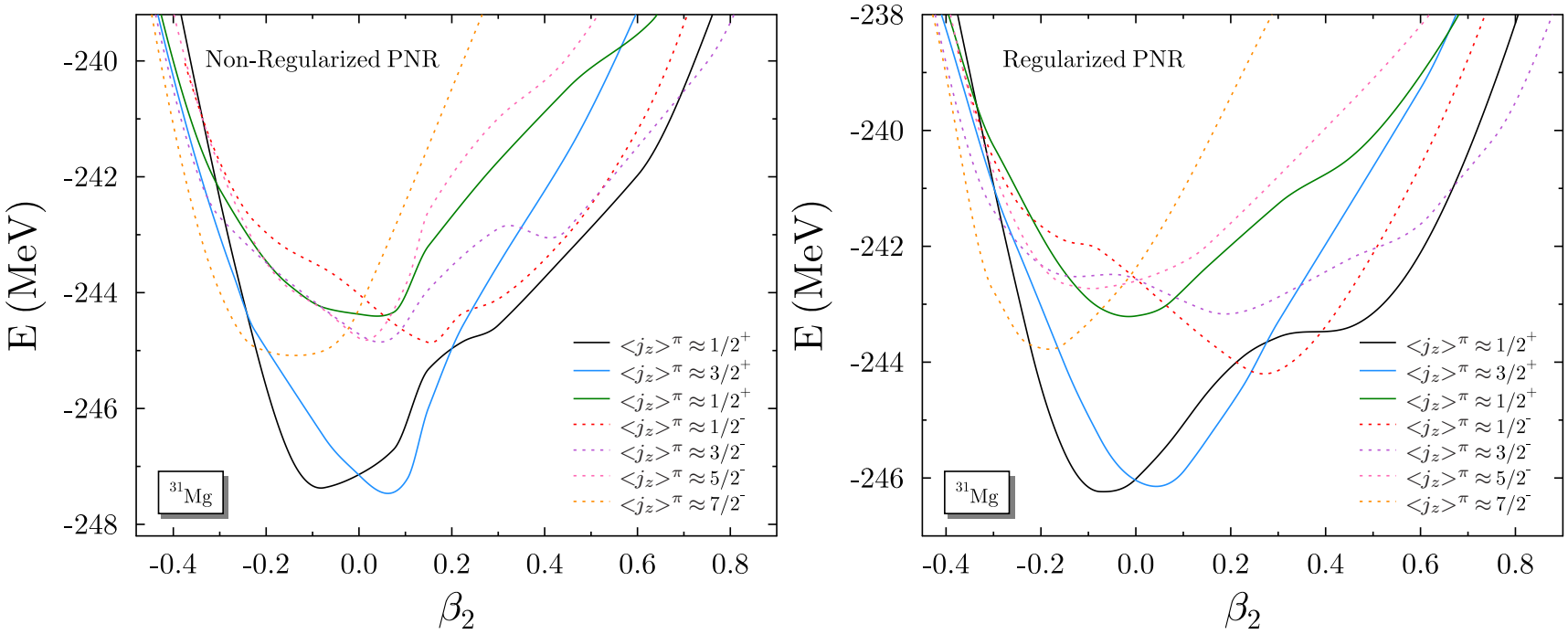




M. B., B. Avez, T. Duguet, P.-H. Heenen, D. Lacroix, unpublished

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

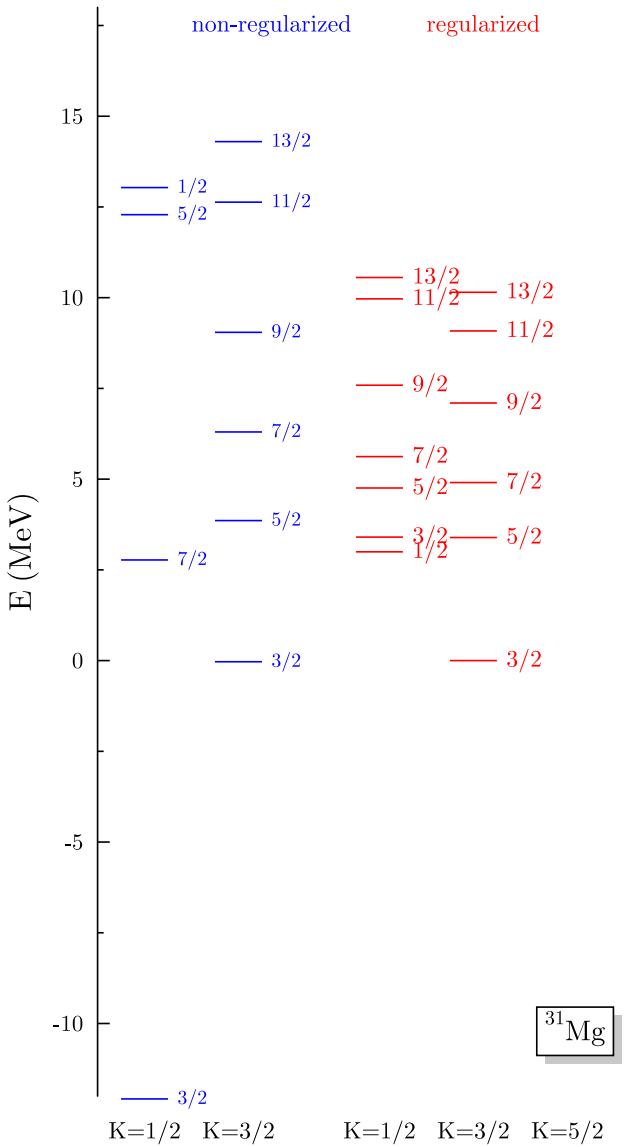
Particle-number restoration of ^{31}Mg



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

All states are constructed as blocked one-quasiparticle HFB states

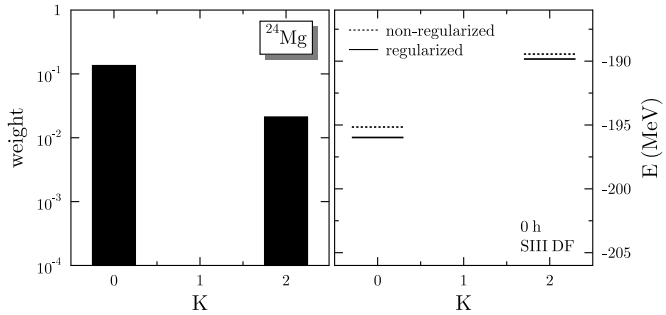
Non-regularized MR EDF with general functionals can give unphysical spectra

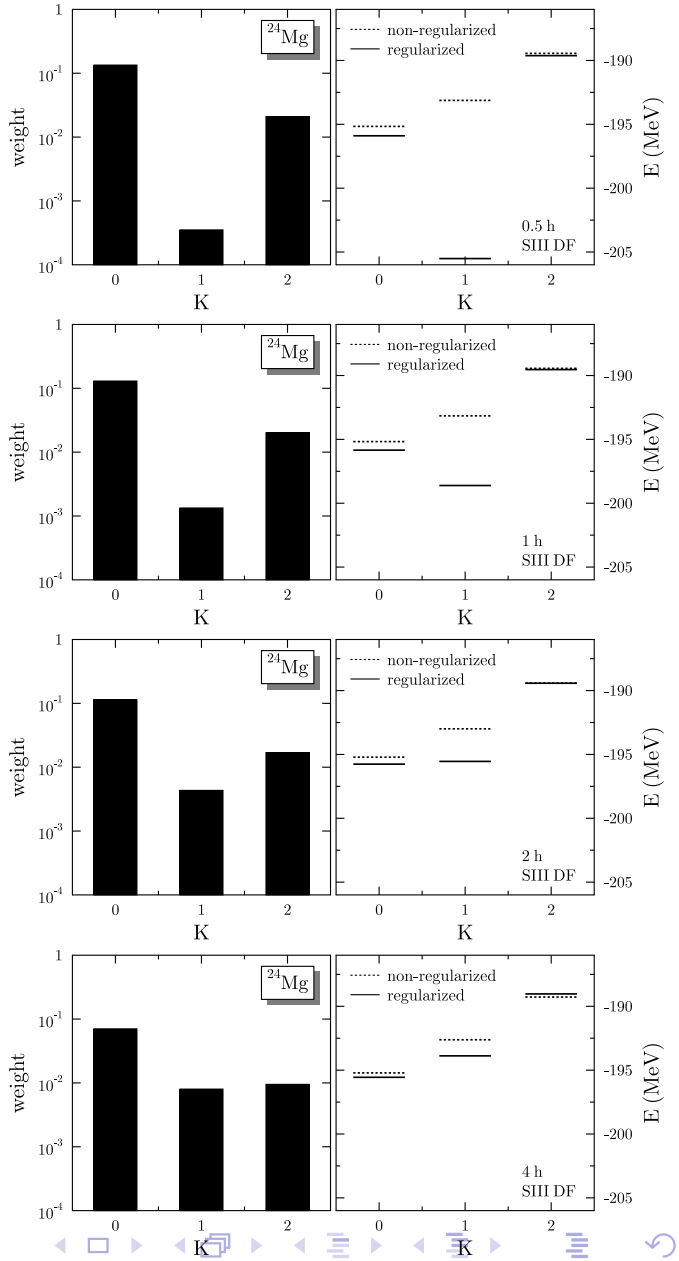


B. Bally, B. Avez, M. B., P.-H. Heenen, unpublished

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

- Non-convergence of combined N and J projection (on a very small scale, though) (not shown)
- 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 vary the size of $K = 1$ components
- example shown in plots: K decomposition in projection on $J = 2$





Again: What to do?

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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

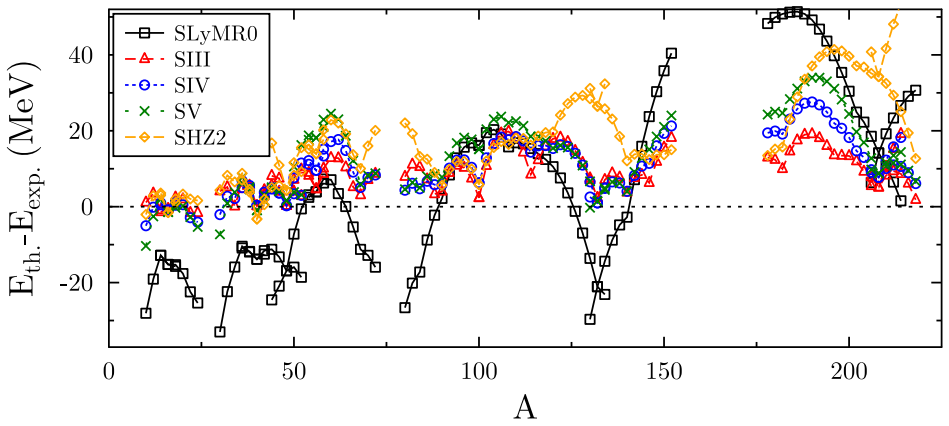
  which was the reason to introduce density dependences etc. in the 1970s.

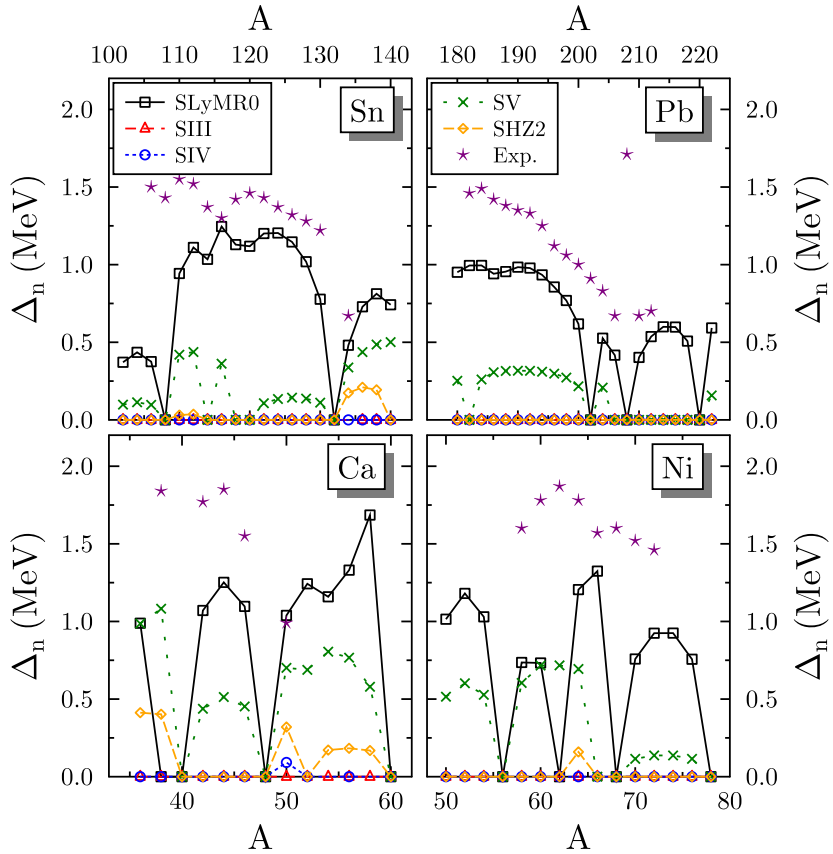
First try: SLyMR0

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

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

First try: standard two-body + gradient-less 3-body & 4-body

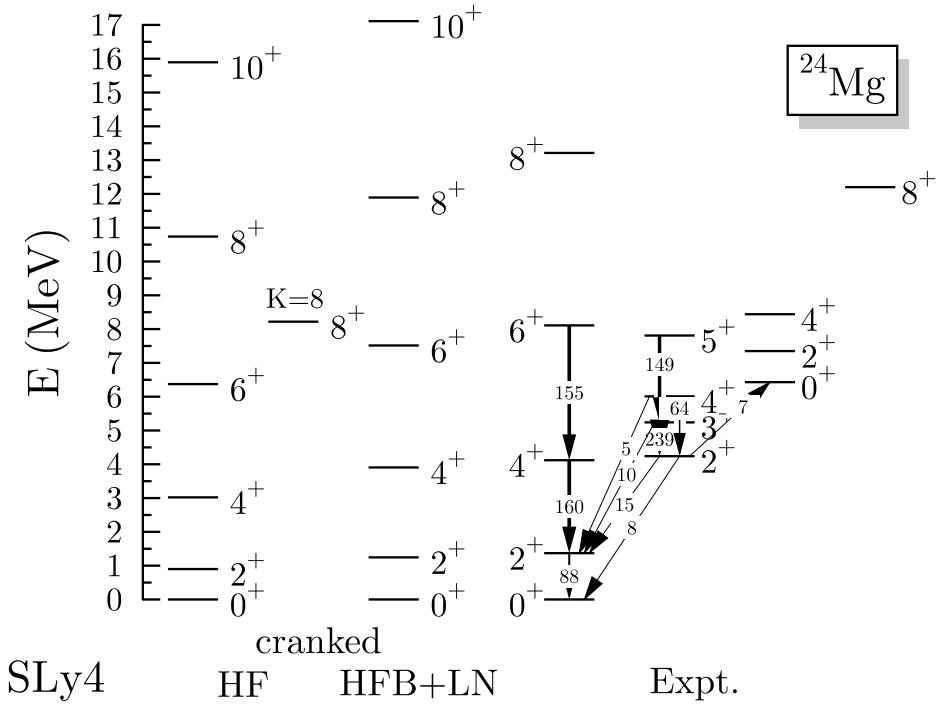




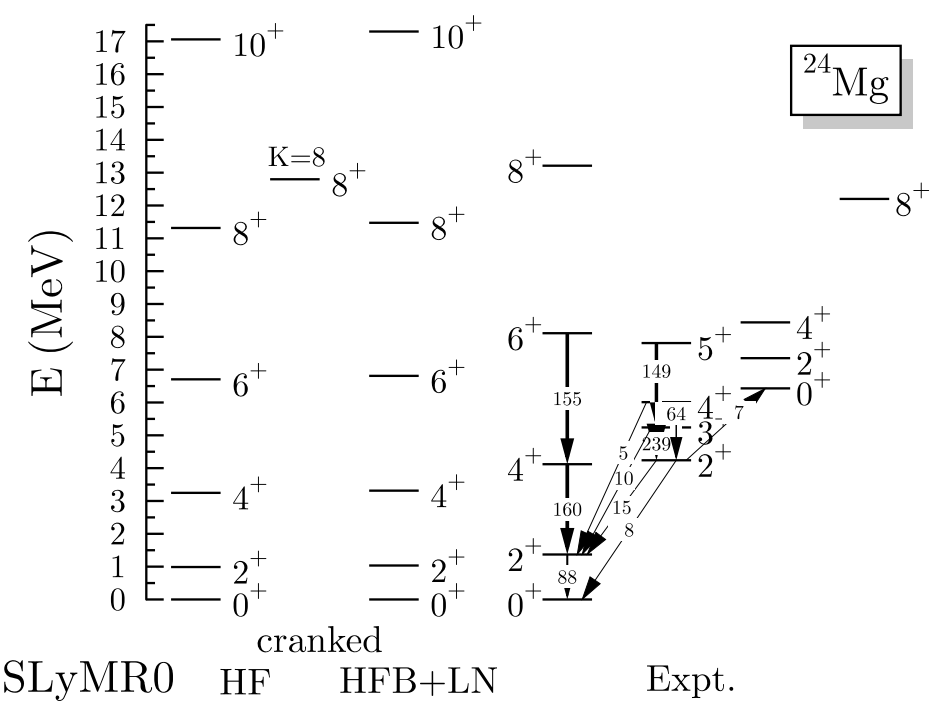
- it is impossible to fullfil the usual nuclear matter constraints , to have stable interactions and attractive pairing
- no "best fit" possible
- very bad performance compared to standard general functionals

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

SR & MR EDF using SLyMR0: the example of ^{24}Mg



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

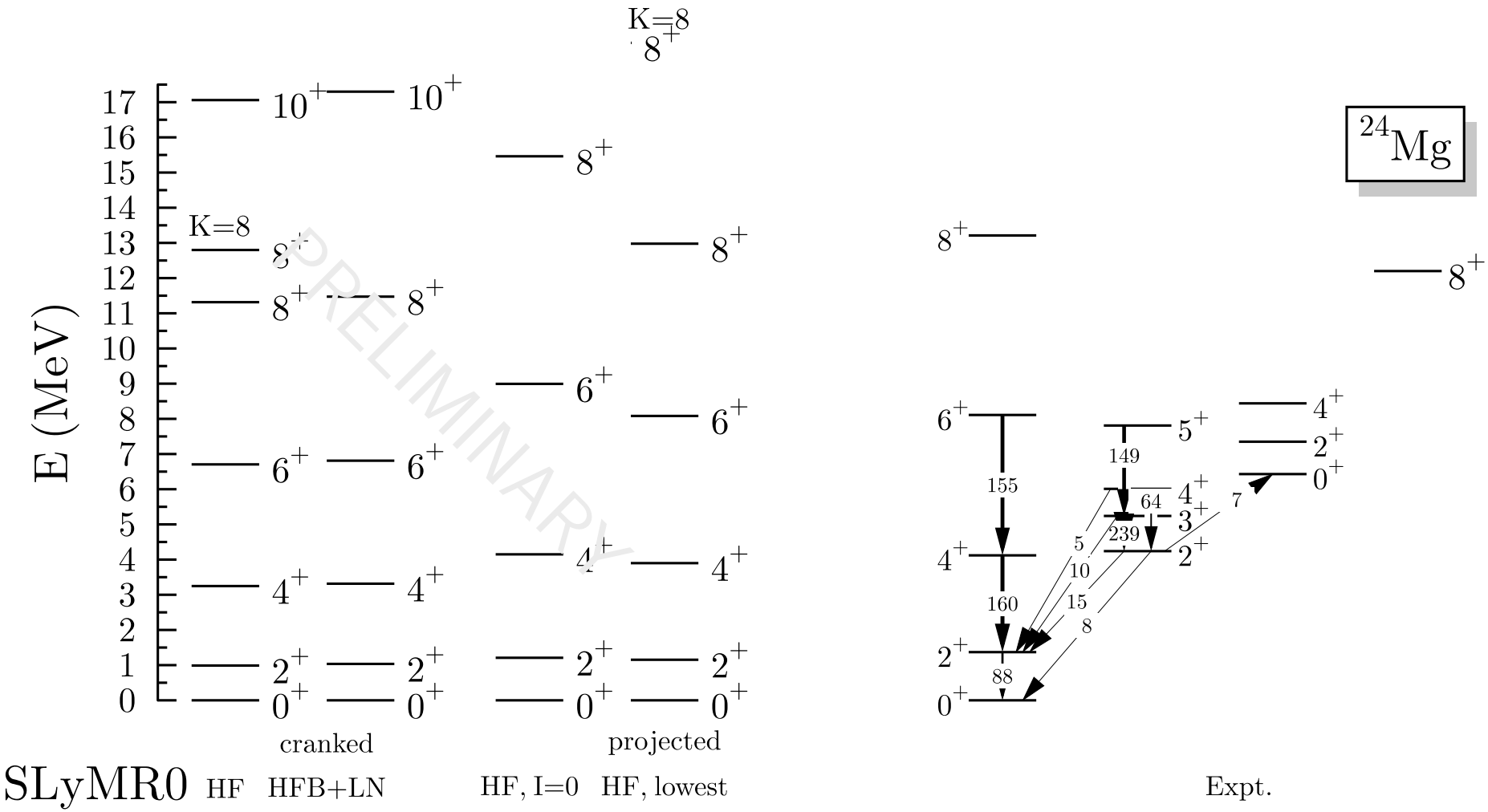


SR EDF (cranked HF & HFB+LN) using SLyMR0

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

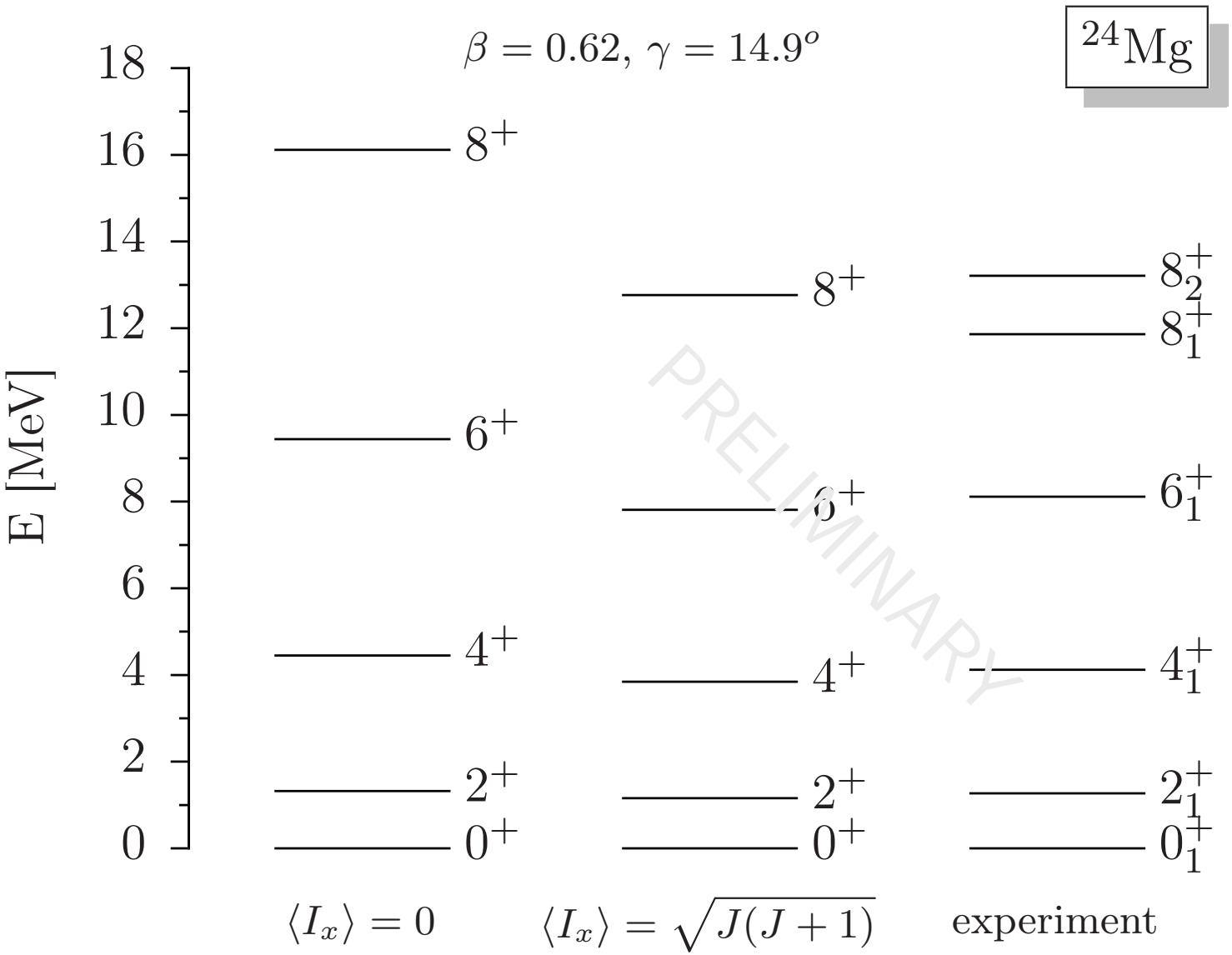
$\Rightarrow$ deformation of HF and HFB+LN is very different for SLyMR0

Decomposition

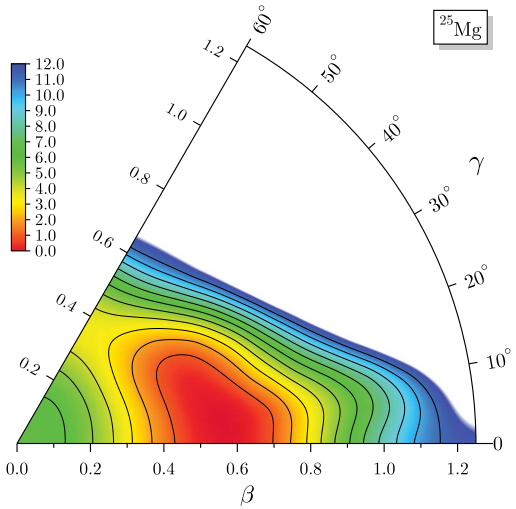


⇒ projection from cranked HFB states compresses the (collective) excitation spectrum

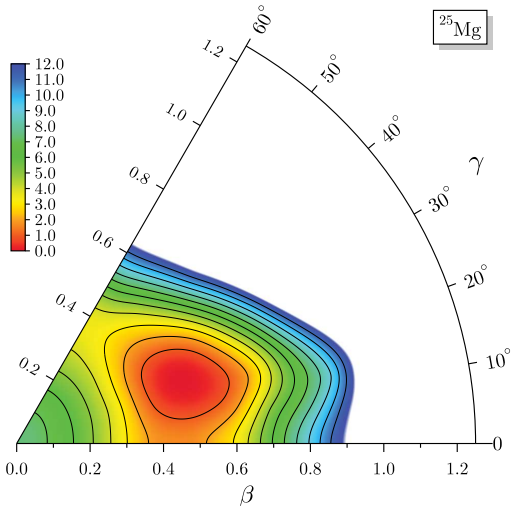
Decomposition



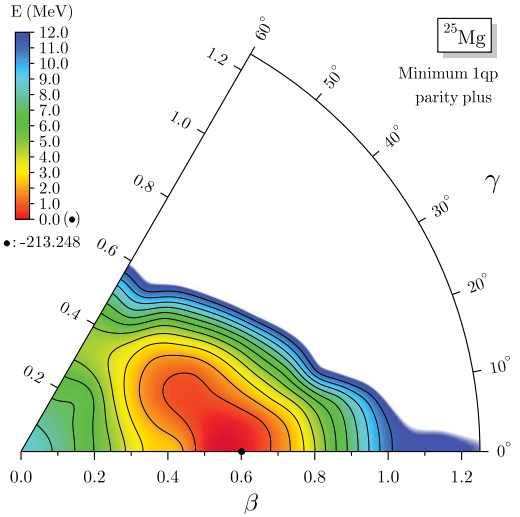
Odd-A nuclei with SLyMR0: The example of ^{25}Mg



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

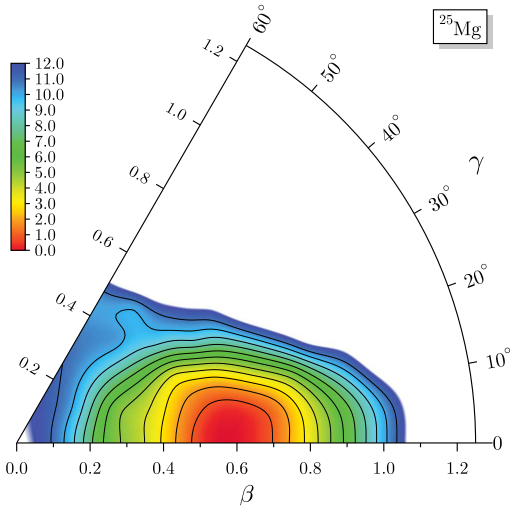


Blocked HFB 1-quasiparticle state, where blocked particle has $\langle j_z \rangle \approx 5/2$



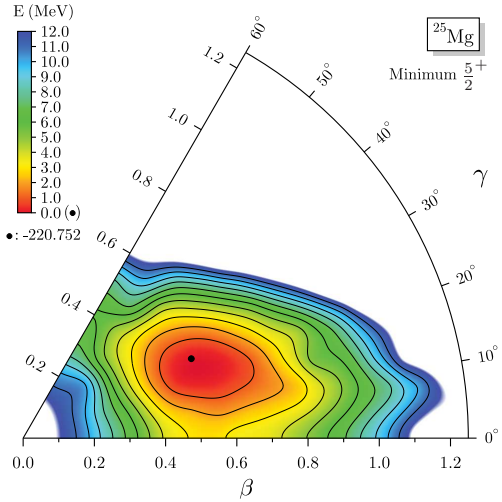
Lowest 1 qp state

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

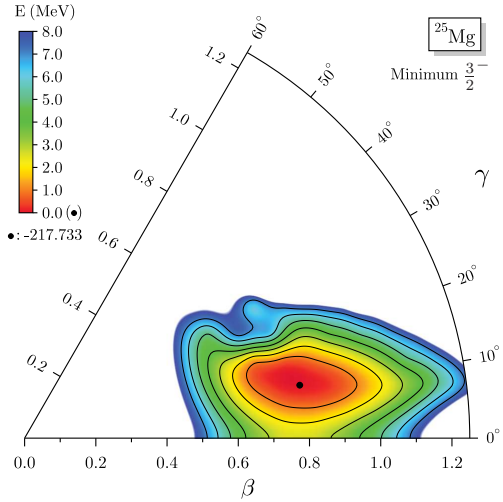


Blocked HFB 1-quasiparticle state, where blocked particle has $\langle j_z \rangle \approx 3/2$

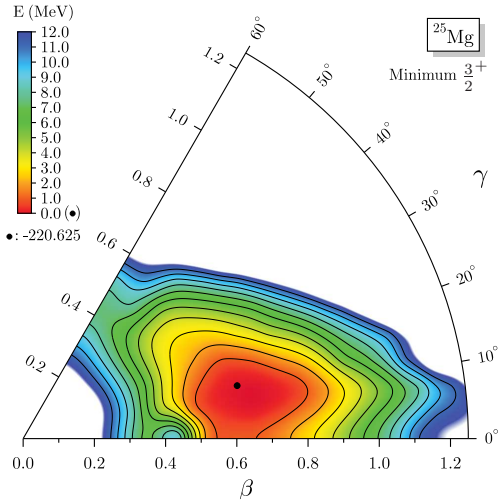
First "beyond-mean-field" results for odd-A nuclei with SLyMR0



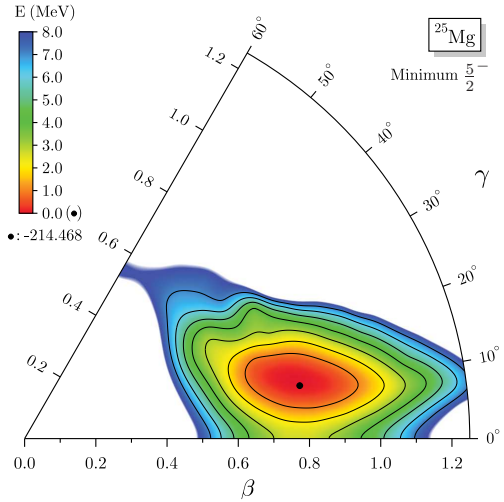
Lowest projected $J = 5/2^+$, $Z = 12$, $N = 13$ state



Lowest projected $J = 3/2^-$, $Z = 12$, $N = 13$ state



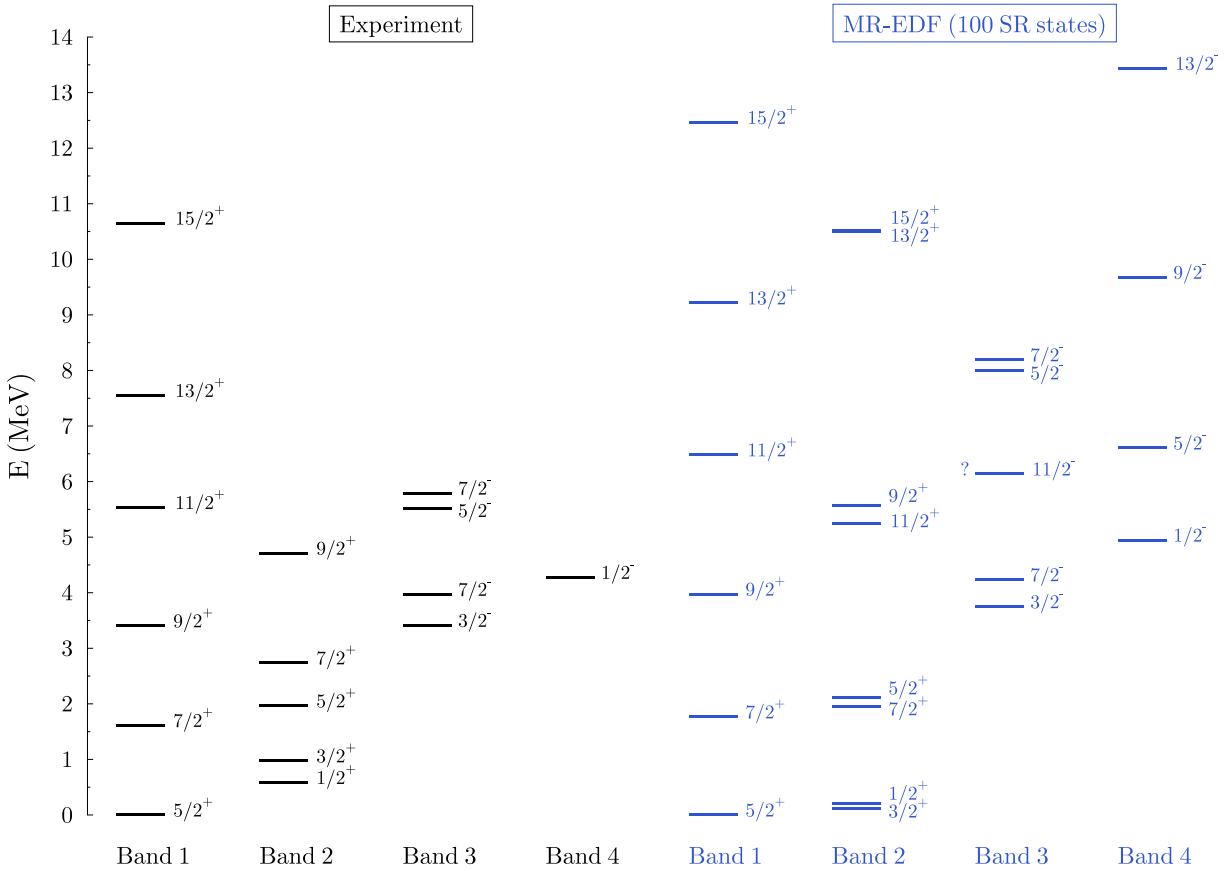
Lowest projected $J = 3/2^+$, $Z = 12$, $N = 13$ state



Lowest projected $J = 5/2^-$, $Z = 12$, $N = 13$ state

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

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

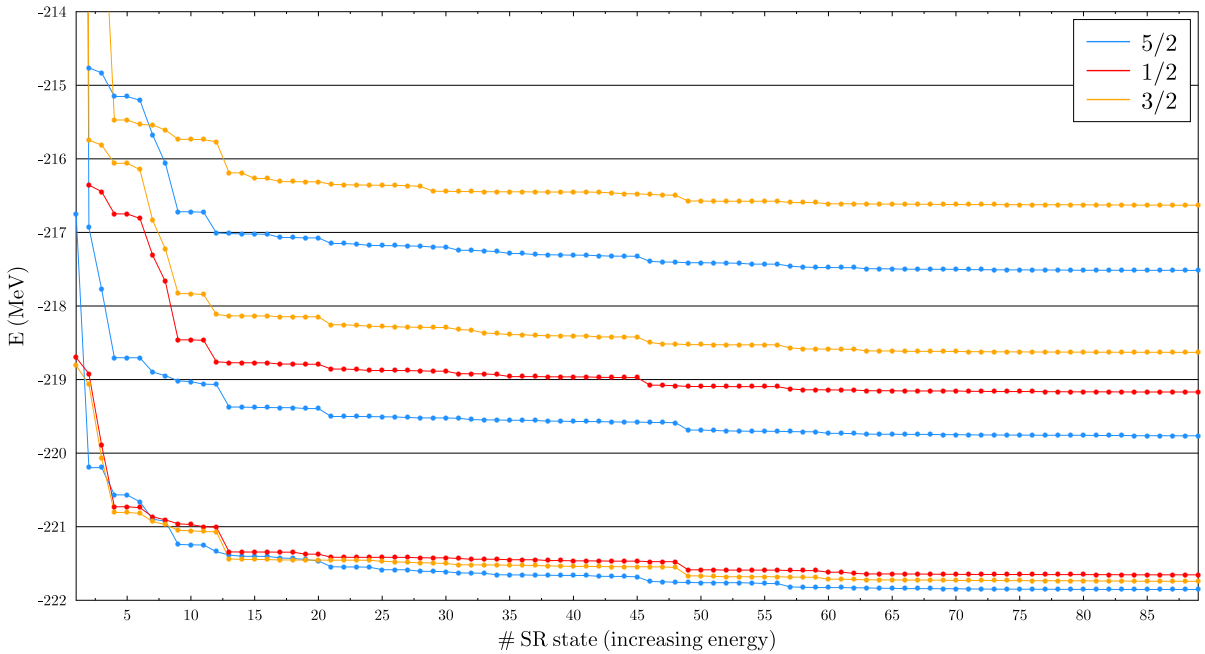


Benjamin Bally, Benoît Avez, M. B., P.-H. Heenen (to be published)

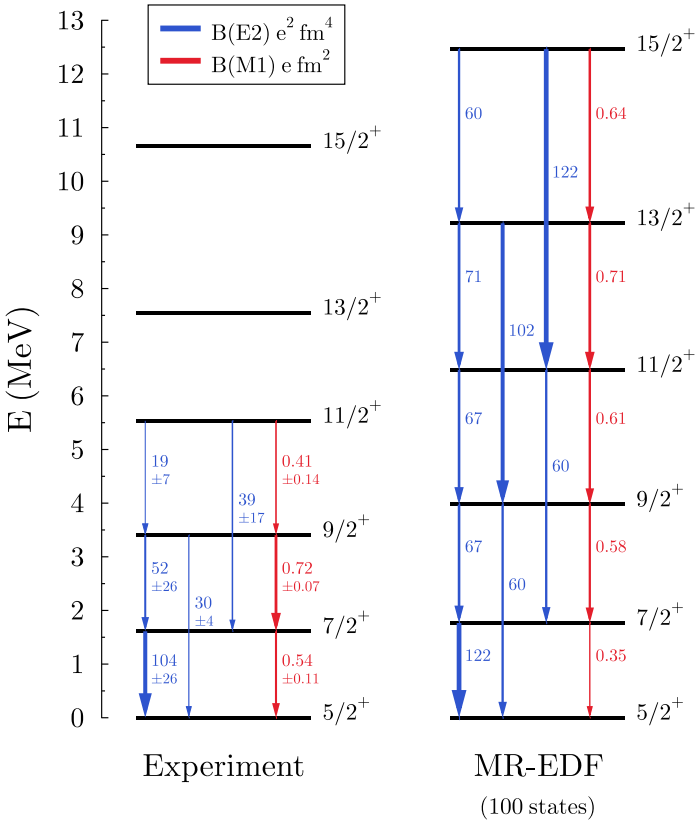
- projected GCM based on 100 blocked 1qp states with positive parity and 60 blocked 1qp states with negative parity
- usually several blocked 1qp states of each parity per deformation
- 6144 non-redundant combinantions of Euler angles, 9×9 gauge angles $\Rightarrow 5 \times 10^7$ states of positive parity, 3×10^7 states of negative parity

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

Convergence of the lowest states with $J^\pi = 1/2^+, 3/2^+, 5/2^+$ when adding states to the basis



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



- "band 1"
- spectroscopic quadrupole moment Q_s of the $5/2^+$ ground state:
  Exp: 20.1 ± 0.3 e fm^2
  Calc: 23.25 e fm^2
- magnetic moment μ of the $5/2^+$ ground state in nuclear magnetons:
  Exp: -0.855
  Calc: -1.054

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

Data from Nuclear Data Sheets 110 (2009) 1691

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

- 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

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

Jeremy Sadoudi, Thomas Duguet, Jacques Meyer, M. B., to be submitted anytime soon

- first preliminary fits underway
- construction of most general spin-orbit + tensor 3-body force of 2nd order in gradients is underway

Take-away messages

- Extension of MR EDF to angular-momentum-optimized reference states
  - improved moments of inertia for high-J collective states
  - collectivity of "non-collective" excited states
  - odd-A nuclei (and, along the same lines, to odd-odd nuclei)
- At time being, there is no known scheme to safely handle general EDFs in a multi-reference framework.
- Using Hamiltonians is the 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.

This research has been brought to you by

The collaboration: (former members who have contributed *in italics*)

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  CEN Bordeaux Gradignan, France
  formalism; beyond-mean-field models; construction of effective interactions; large-scale applications
- K. Bennaceur, D. Davesne, R. Jodon, J. Meyer, *A. Pastore*
  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