Beyond mean-field description of nuclear properties

- Basis of the method: symmetry restoration and mixing on deformation
- Analysis of the generator coordinate method in ^{46}Ca, triaxial shapes and 2qp excitations
- Application to an odd nucleus ^{25}Mg
- Octupole deformations

- Collaboration with M. Bender (CENBG)
- Contributors:

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  CENBG: B. Avez, B. Bally and J. Sadoudi

  IPNL, Lyon: K. Bennaceur and R. Jodon

Symmetry restoration + configuration mixing on HFB wave functions

(i) First step: vacuum or “false vacuum”

$$|\mathrm{HFB}_{\mathrm{fv}}(q_1,q_2)\rangle = \prod_{k>0}(u_k + v_k a_k^\dagger a_{\bar{k}}^\dagger)|-\rangle,$$

Constraint on N and Z but no qp excitation.
Put the Fermi energy at the right place.

(ii) Second step: several 1qp or 2qp states are calculated self-consistently for each (q1,q2) or (q1,q3)

(iii) For each state, restoration of symmetry and K-mixing (or parity)

$$|J^\pi M \kappa(\mu)\rangle = \sum_{K=-J}^{J} f_{\mu,K}^{J^\pi \kappa}\, \hat{P}^J_{MK} \hat{P}^N \hat{P}^Z |\mathrm{HFB}^\pi_{1\mathrm{qp}}(\mu)\rangle$$

The coefficients *f* are determined by the HWG equation:

$$\sum_{K'} \left(\mathcal{H}^{J^\pi}_{\mu,K;\mu,K'} - E^{J^\pi}_{\kappa} \mathcal{I}^{J^\pi}_{\mu,K;\mu,K'} \right) f^{J^\pi \kappa}_{\mu,K'} = 0$$

It requires to calculate the overlap and Hamiltonian kernels:

$$\mathcal{I}^{J^\pi}_{\mu,K;\mu',K'} \equiv \langle \mathrm{HFB}^\pi_{1\mathrm{qp}}(\mu)|\hat{P}^J_{KK'}\hat{P}^Z\hat{P}^N|\mathrm{HFB}^\pi_{1\mathrm{qp}}(\mu')\rangle$$

$$\mathcal{H}^{J^\pi}_{\mu,K;\mu',K'} \equiv \langle \mathrm{HFB}^\pi_{1\mathrm{qp}}(\mu)|H P^J_{KK'}P^Z P^N|\mathrm{HFB}^\pi_{1\mathrm{qp}}(\mu')\rangle$$

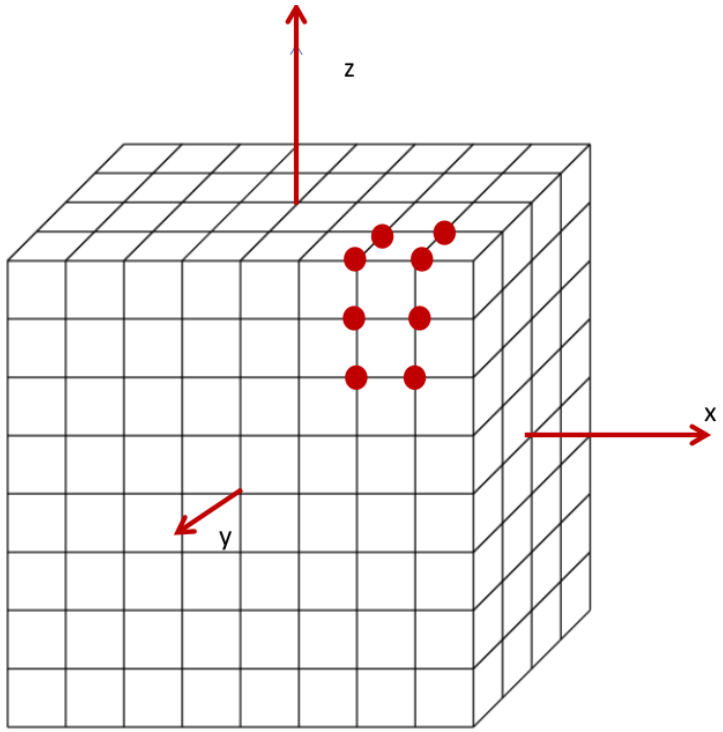
(iiii) Last step: configuration mixing on the quadrupole deformation (q_1 q_2) of all the states projected on (JM, N, Z). Several states for each deformation!

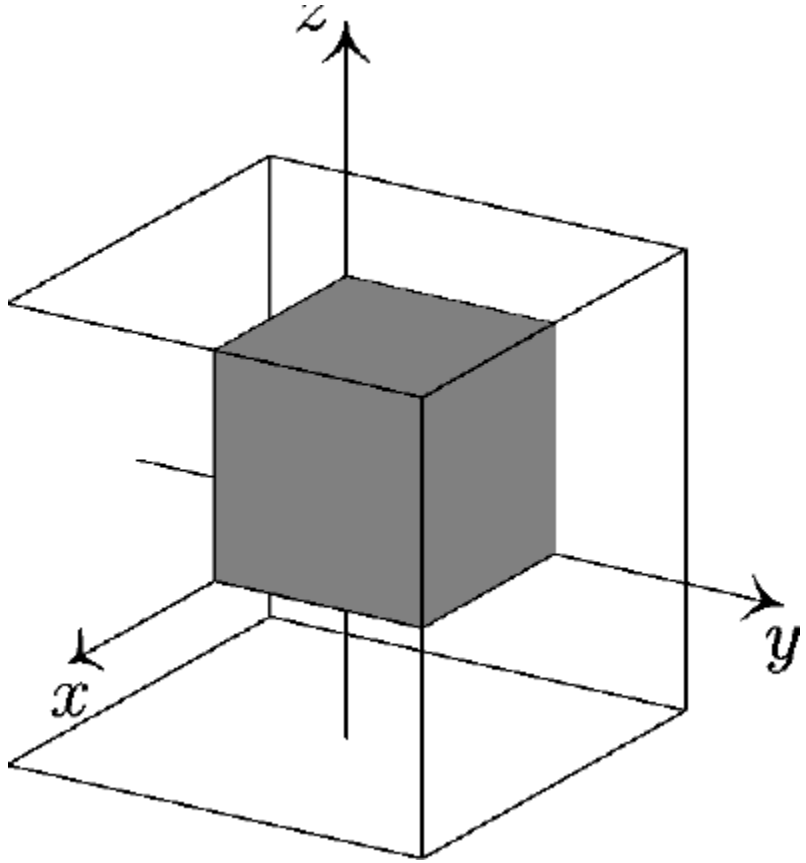
$$|J^\pi M\xi\rangle = \sum_{\mu=1}^{\Omega_I}\sum_{\kappa} f^{J^\pi\xi}_{\mu,\kappa}\,|J^\pi M\kappa(\mu)\rangle$$

At steps 3 and 4, removal of states corresponding to small values of the norm or to non-accurate values of $\langle J^2\rangle$

The numerical technique: discretization on a 3-dimensional mesh

Lagrange derivatives (J. Phys. A 19 2041 (1986))
Numerical accuracy of the order of 10 keV





For ^{25}Mg and ^{46}Mg , use of the same forces in the mean-field and pairing channels SLyMR0 and SLyMR1

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

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

Coulomb direct and exchange calculated exactly

The principles of the generator coordinate method

-non orthogonal basis depending on parameters α:

$$\langle \alpha | \alpha' \rangle \;=\; \mathcal{I}(\alpha, \alpha') \neq \delta_{\alpha\alpha'}$$

$$\mathcal{H}(\alpha, \alpha') \;=\; \langle \alpha | \hat{H} | \alpha' \rangle$$

- New wave functions

$$|\mu\rangle \;=\; \sum_{\alpha=1}^{\Omega_\alpha} f_\mu(\alpha) |\alpha\rangle$$

-The f_μ are obtained by minimizing the energy:

$$\sum_{\alpha'=1}^{\Omega_\alpha} \left[\mathcal{H}(\alpha, \alpha') - E_\mu \, \mathcal{I}(\alpha, \alpha') \right] \, f_\mu(\alpha') = 0.$$

- They are non orthogonal

$$\sum_{\alpha, \alpha'=1}^{\Omega_\alpha} f^*_{\mu'}(\alpha) \, \mathcal{I}(\alpha, \alpha') \, f_\mu(\alpha') = 0 \qquad \text{for } \mu \neq \mu'$$

Not the right basis to solve the HWG equation and to define a collective wave function

Better to define a new wave-function:

$$g_\mu(\alpha) = \sum_{\alpha'=1}^{\Omega_\alpha} \mathcal{I}^{1/2}(\alpha,\alpha')\, f_\mu(\alpha')$$

$$\tilde{H}(\alpha,\alpha') = \sum_{\alpha'',\alpha'''=1}^{\Omega_\alpha} \mathcal{I}^{-1/2}(\alpha,\alpha'')\, \mathcal{H}(\alpha'',\alpha''')\, \mathcal{I}^{-1/2}(\alpha''',\alpha')$$

One ends up with a more convenient problem

$$\sum_{\alpha'=1}^{\Omega_\alpha} \tilde{H}(\alpha,\alpha')\, g_\mu(\alpha') = E_\mu\, g_\mu(\alpha)\,.$$

However: very redundant basis!

To identify nearly redundant states, diagonalization of the norm kernel $\mathcal{I}$:

$$\sum_{\alpha,\alpha'=1}^{\Omega_\alpha} u_n(\alpha)\,\mathcal{I}(\alpha,\alpha')\,u_{n'}(\alpha') = \lambda_n\,\delta_{nn'}$$

$$|n\rangle = \frac{1}{\sqrt{\lambda_n}}\,u_n(\alpha)\,|\alpha\rangle$$

Change to the basis formed by the norm eigenstates and elimination of vectors corresponding to small eigenvalues

$$g_\mu(n) = \sqrt{\lambda_n}\sum_{\alpha=1}^{\Omega_\alpha} u_n(\alpha)\,f_\mu(\alpha)$$

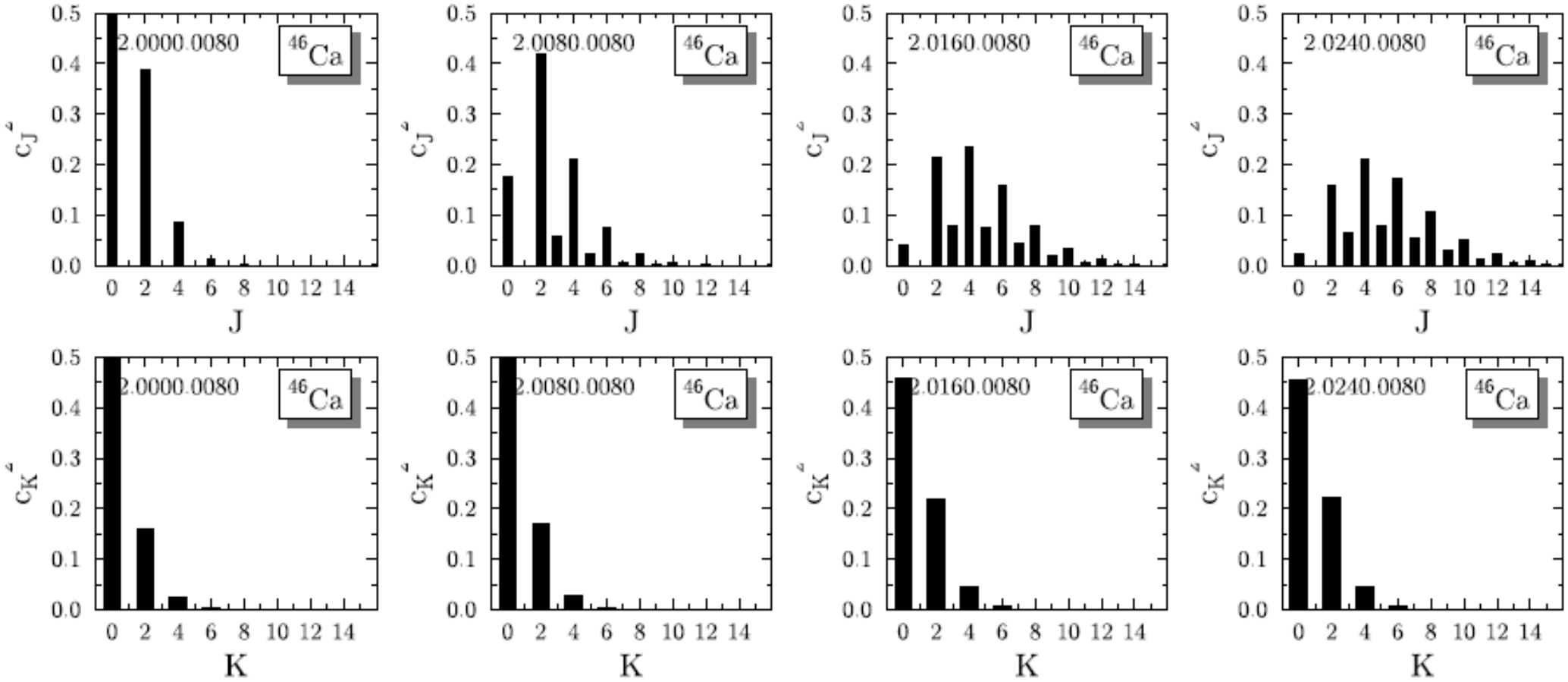
$$\tilde{H}(n,n') = \frac{1}{\sqrt{\lambda_n\,\lambda_{n'}}}\sum_{\alpha,\alpha'=1}^{\Omega_\alpha} u_n(\alpha)\,\mathcal{H}(\alpha,\alpha')\,u_{n'}(\alpha')$$

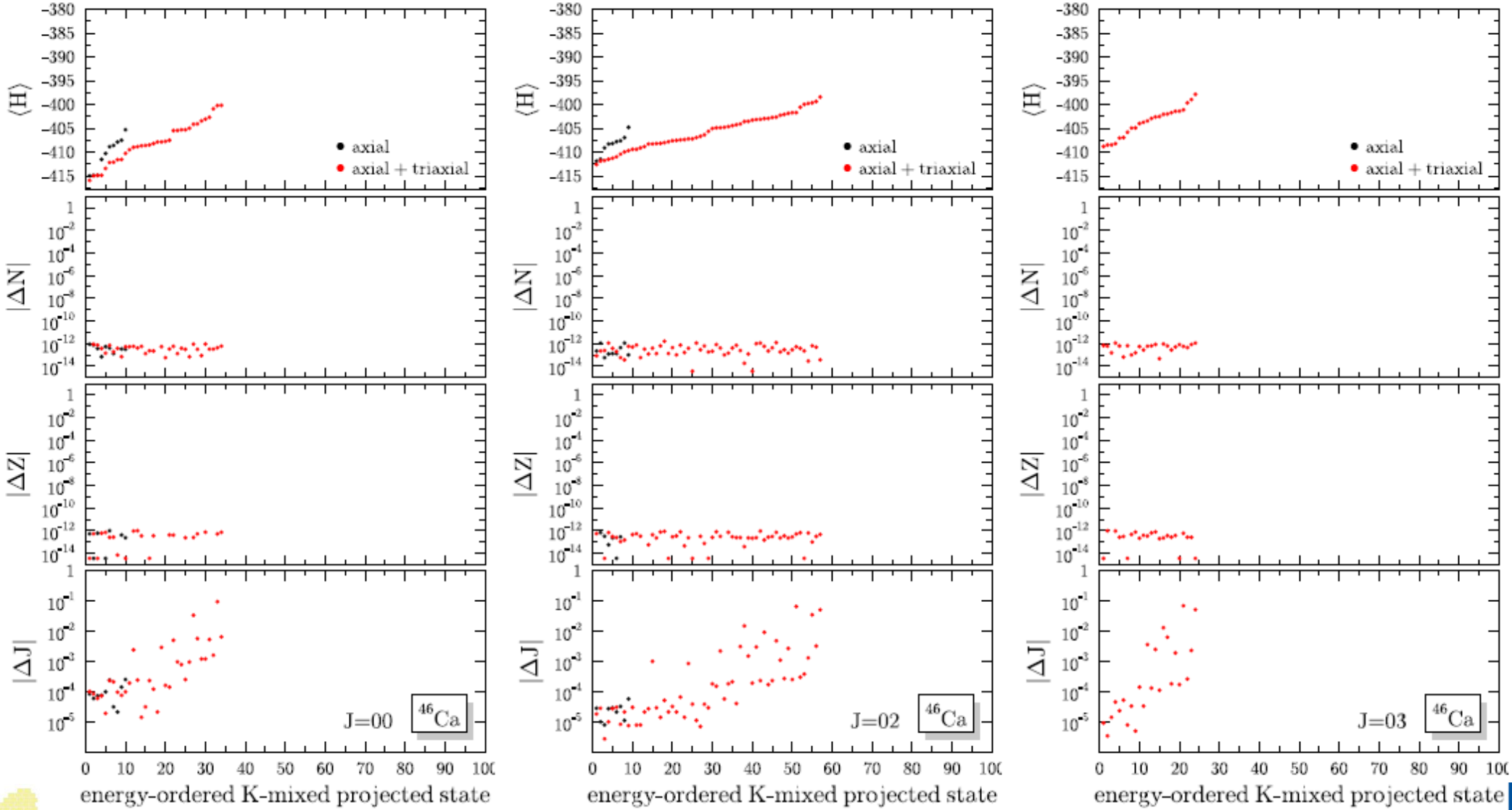
$$\sum_{n=1}^{\Omega_n} \tilde{H}(n',n)\,g_\mu(n) = E_\mu\,g_\mu(n')\,.$$

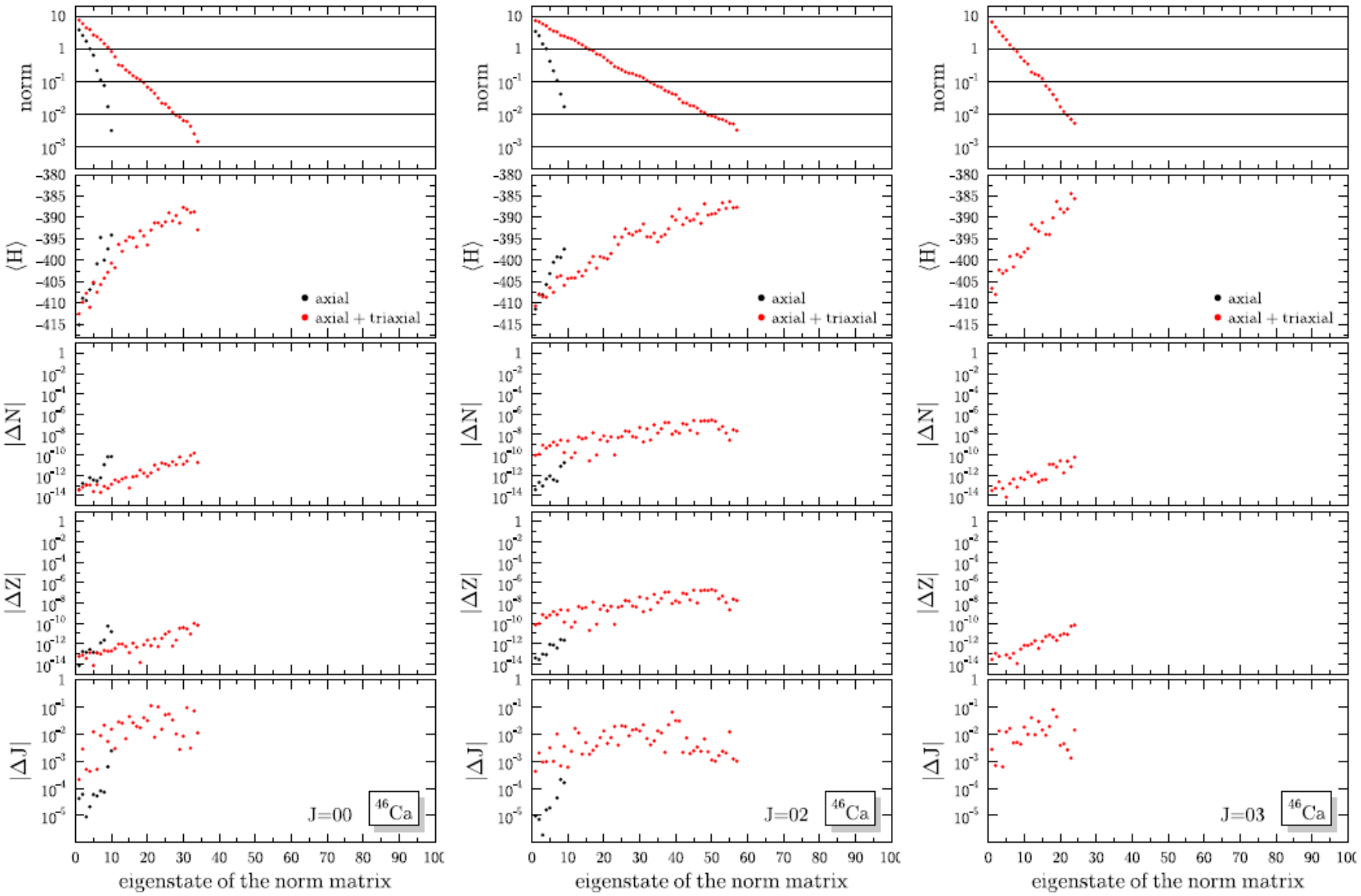
One can go back to the original bases from these eigenstates
Relations not exact anymore if small norm states are removed!

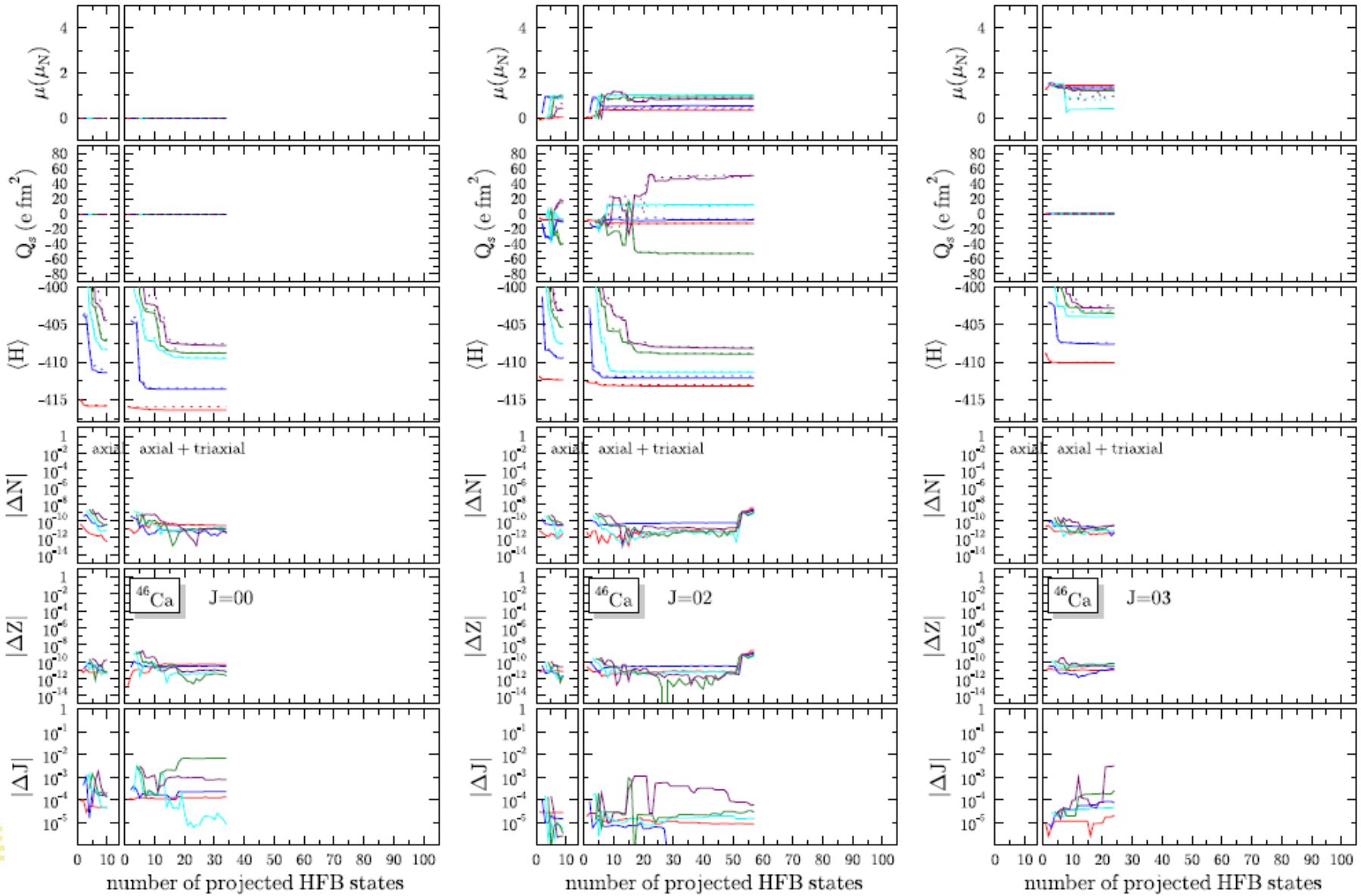
At each step in red, selection of states

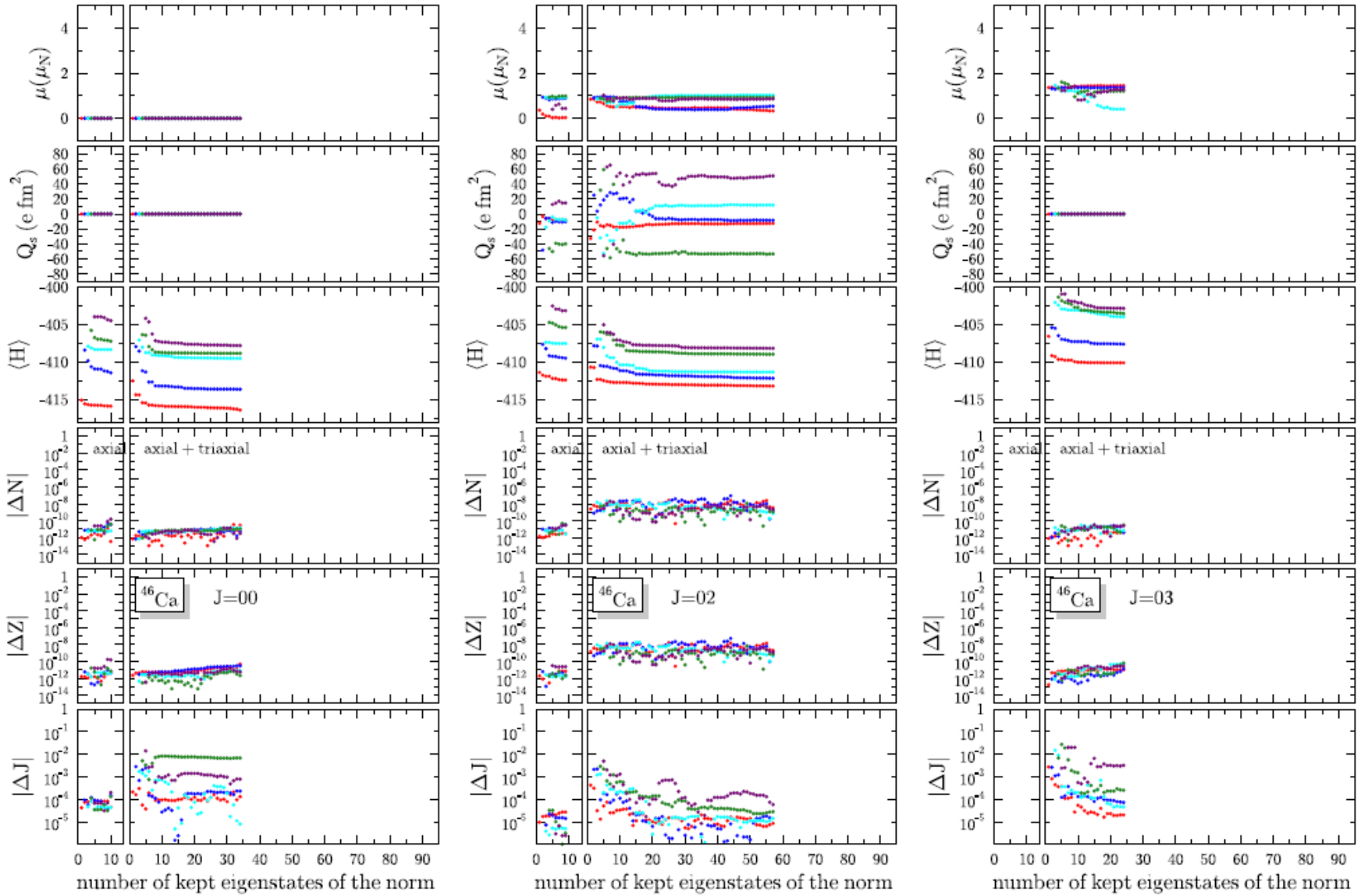
- (i) First step: vacuum or “false vacuum”
- (ii) Second step: several 1qp or 2qp states are calculated self-consistently for each (q1,q2)
- For each state, restoration of symmetry
- K-mixing
- configuration mixing on the quadrupole deformation (q_1 q_2) of all the states projected on (JM, N, Z).


2.0000.0080
2.0080.0080
2.0160.0080
2.0240.0080
46Ca
cJ2
cK2
J
K
0.0
0.1
0.2
0.3
0.4
0.5
0 2 4 6 8 10 12 14


⟨H⟩
axial
axial + triaxial
|ΔN|
|ΔZ|
|ΔJ|
J=00
J=02
J=03
^{46}Ca
energy-ordered K-mixed projected state


norm
⟨H⟩
axial
axial + triaxial
|ΔN|
|ΔZ|
|ΔJ|
J=00
J=02
J=03
46Ca
eigenstate of the norm matrix

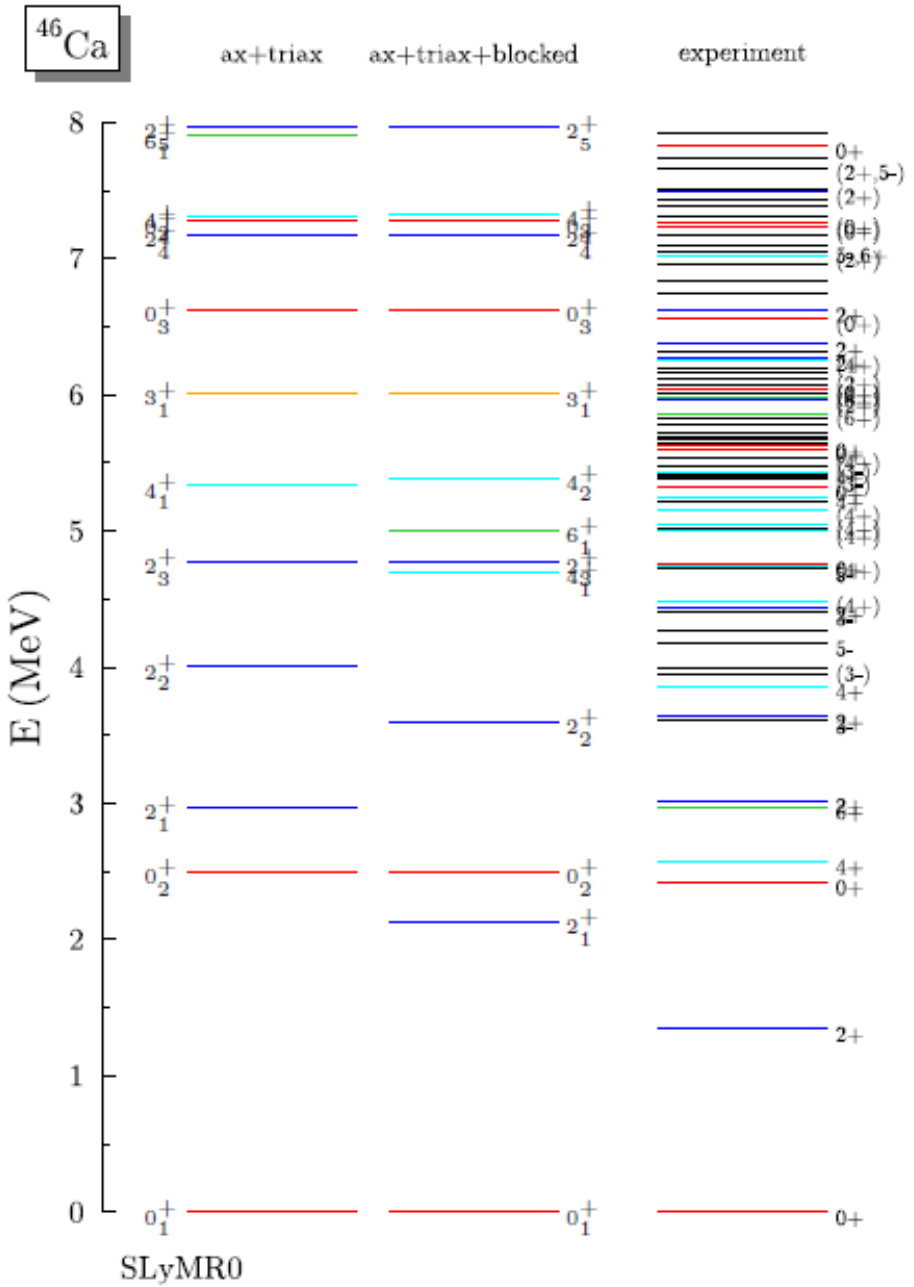

$\mu(\mu_N)$
Q_s (e fm^2)
⟨H⟩
|ΔN|
|ΔZ|
|ΔJ|
axial
axial + triaxial
^{46}Ca
J=00
J=02
J=03
number of projected HFB states


μ(μN)
Qs (e fm2)
⟨H⟩
|ΔN|
|ΔZ|
|ΔJ|
axial
axial + triaxial
46Ca J=00
46Ca J=02
46Ca J=03
number of kept eigenstates of the norm

Adding 2qp excitations

Construction of a few 2qp excitations without (q1,q2) constraints
At the end, 3 are relevant (energy low enough):

		J=2	3	4	5	6	7	8	energy		
$1/2^- + 3/2^-$	K=2	0.38	0.02	0.25	0.01	0.17	0.01	0.01	2^+ lowest	4^+	6^+
$1/2^- + 7/2^-$	K=4	10^{-5}	10^{-5}	0.28	0.01	0.59	0.01	0.01	6^+ lowest	4^+	
$5/2^- + 7/2^-$	K=6	10^{-5}	10^{-6}	10^{-5}	10^{-6}	0.89	0.02	0.01	6^+ lowest		


46Ca
ax+triax
ax+triax+blocked
experiment
E (MeV)
SLyMR0

^{25}Mg

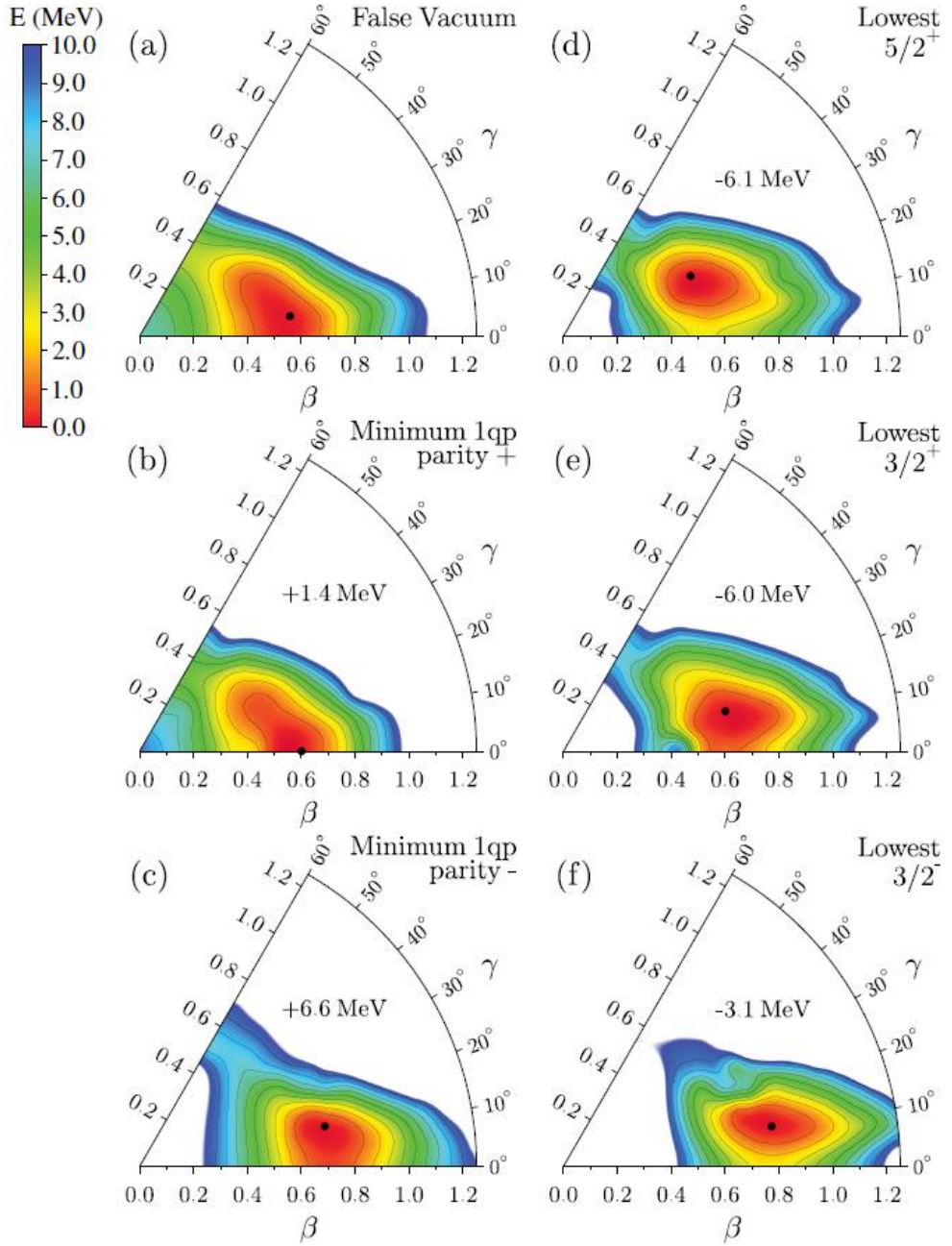
Size of the basis:

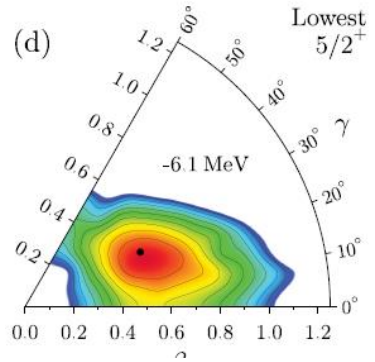
- Points in the triaxial plane every 40 fm^2 (around 30 points)
- 604 1qp states of positive parity
- 222 1qp states of negative parity

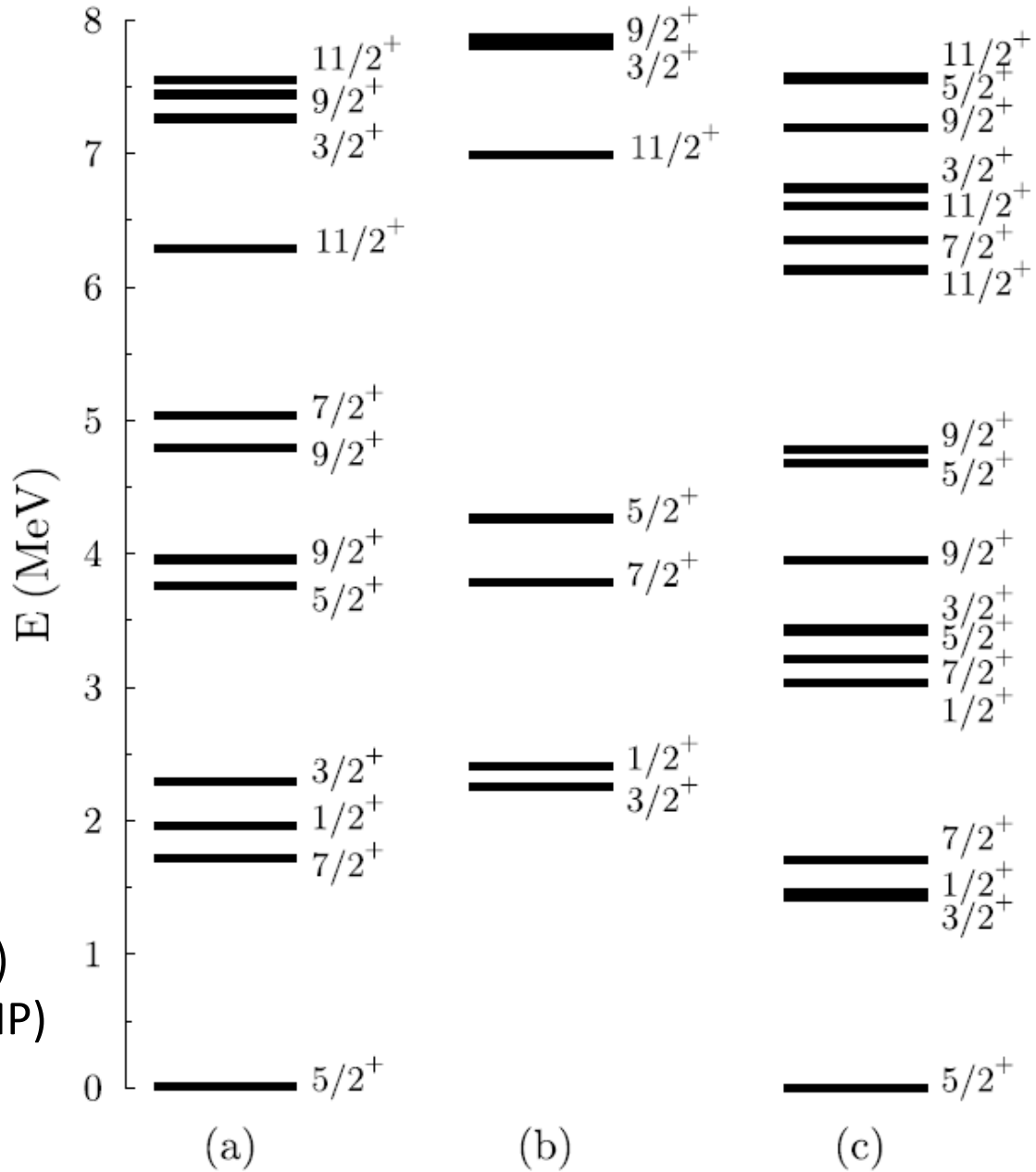
- Selection on energy between all these states, finally 100 and 60 states selected for projection and configuration mixing.

- After K-mixing, each of these 1 qp states can generate several states for each J-value.
- Final dimension of the bases: 226 for $5/2^+$
  149 for $3/2^+$
  106 for $3/2^-$

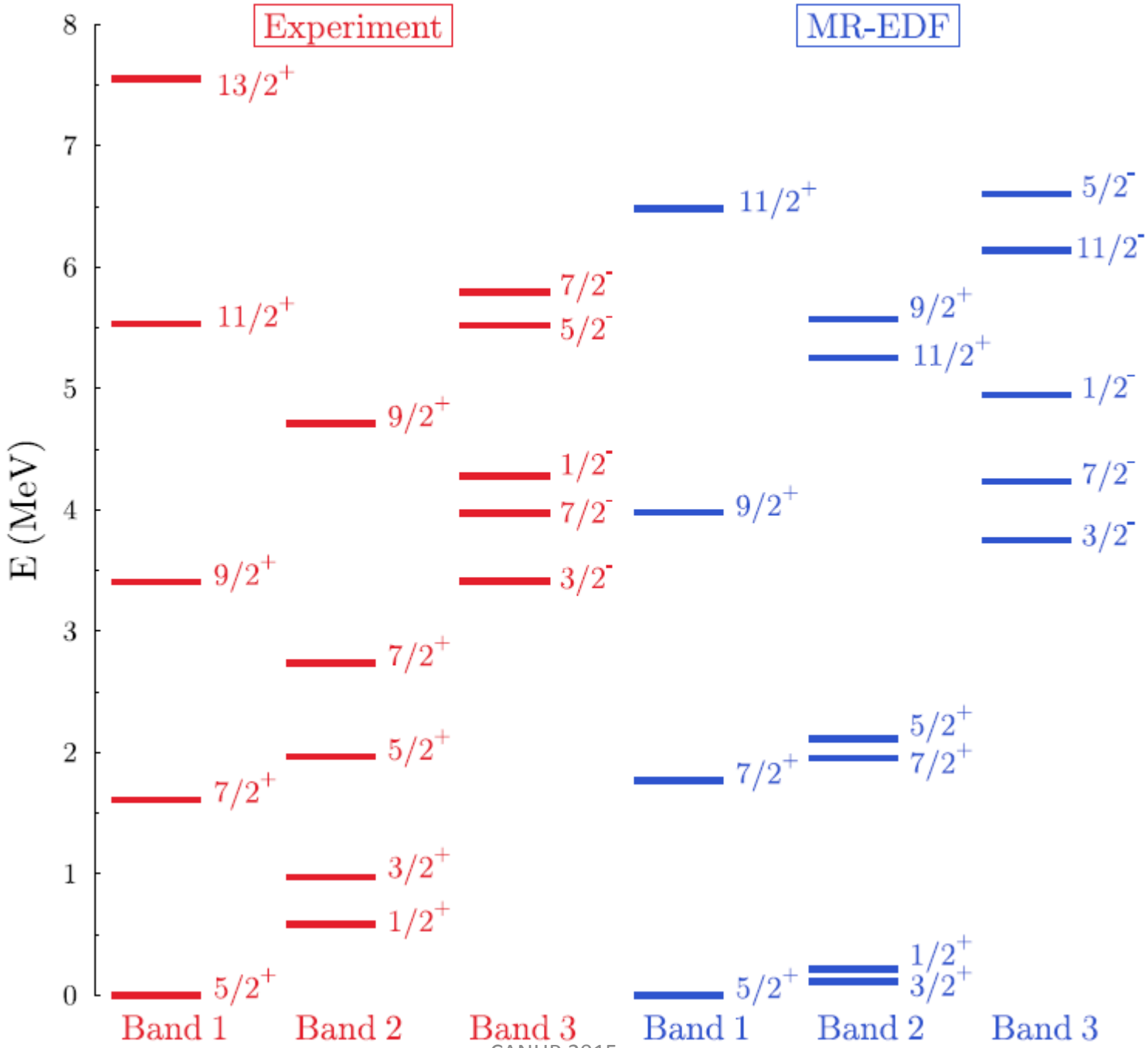
- Accuracy around 20 keV

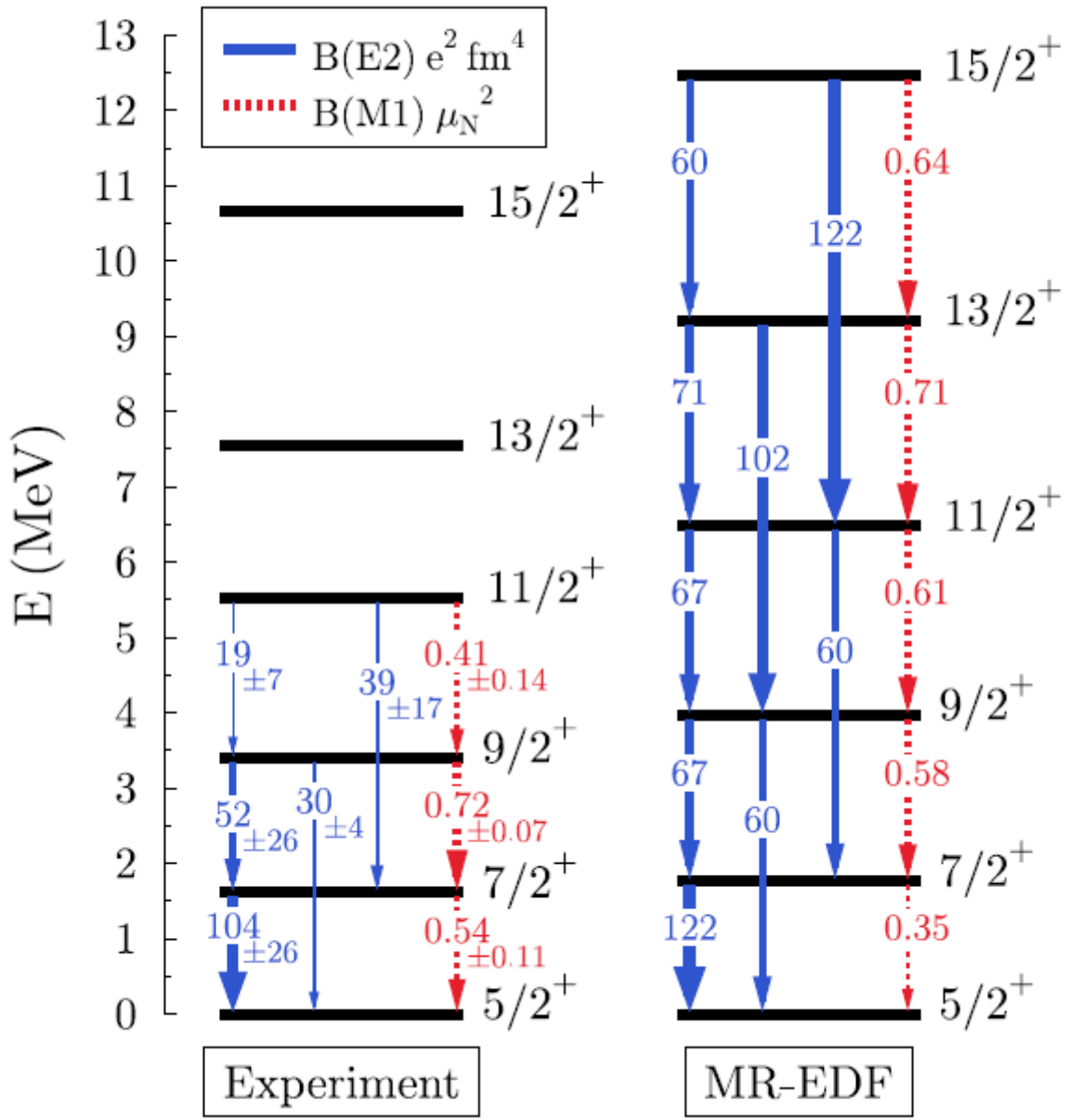

E (MeV)
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
(a) False Vacuum
(b) Minimum 1qp parity +
(c) Minimum 1qp parity -
(d) Lowest 5/2+
-6.1 MeV
(e) Lowest 3/2+
-6.0 MeV
(f) Lowest 3/2-
-3.1 MeV
+1.4 MeV
+6.6 MeV
β
γ





Change in energy different
for each states:
1qp states differ by 4.8 MeV
3.2 MeV (PNP)
2.2 MeV (+AMP)


Experiment
MR-EDF
E (MeV)
0
1
2
3
4
5
6
7
8
$13/2^+$
$11/2^+$
$9/2^+$
$7/2^+$
$5/2^+$
$7/2^-$
$5/2^-$
$1/2^-$
$3/2^-$
$3/2^+$
$1/2^+$
$11/2^+$
$9/2^+$
$7/2^+$
$5/2^+$
$5/2^-$
$11/2^-$
$1/2^-$
$7/2^-$
$3/2^-$
$5/2^+$
$7/2^+$
$1/2^+$
$3/2^+$
Band 1
Band 2
Band 3
Band 1
Band 2
Band 3

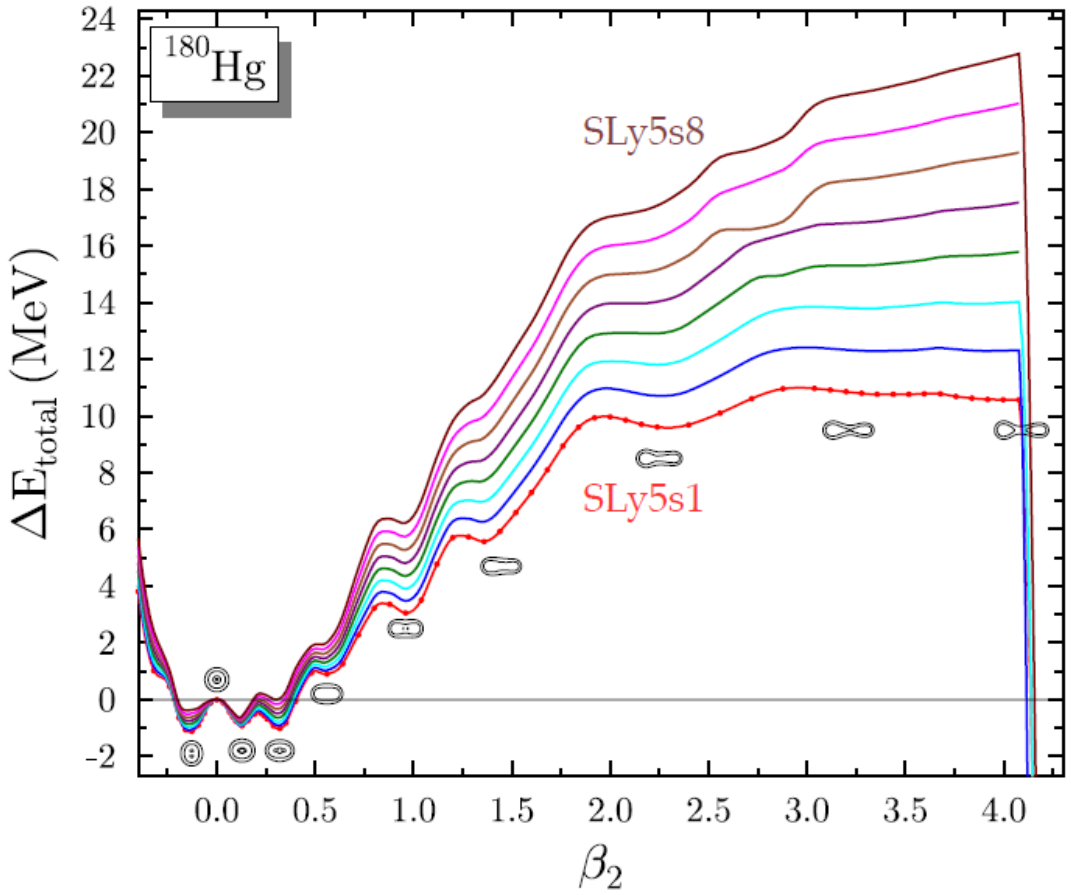

B(E2) e^2 fm^4
B(M1) $\mu_N{}^2$
E (MeV)
13
12
11
10
9
8
7
6
5
4
3
2
1
0
$15/2^+$
$13/2^+$
$11/2^+$
$9/2^+$
$7/2^+$
$5/2^+$
19 ±7
39 ±17
0.41 ±0.14
52 ±26
30 ±4
0.72 ±0.07
104 ±26
0.54 ±0.11
Experiment
60
122
0.64
71
102
0.71
67
60
0.61
67
60
0.58
122
0.35
MR-EDF

Octupole deformations

- Same formalism: two shape degrees of freedom, axial quadrupole and octupole
- EDF instead of force (SLy5 or a variant)
- Projection on parity together with projection on J, M

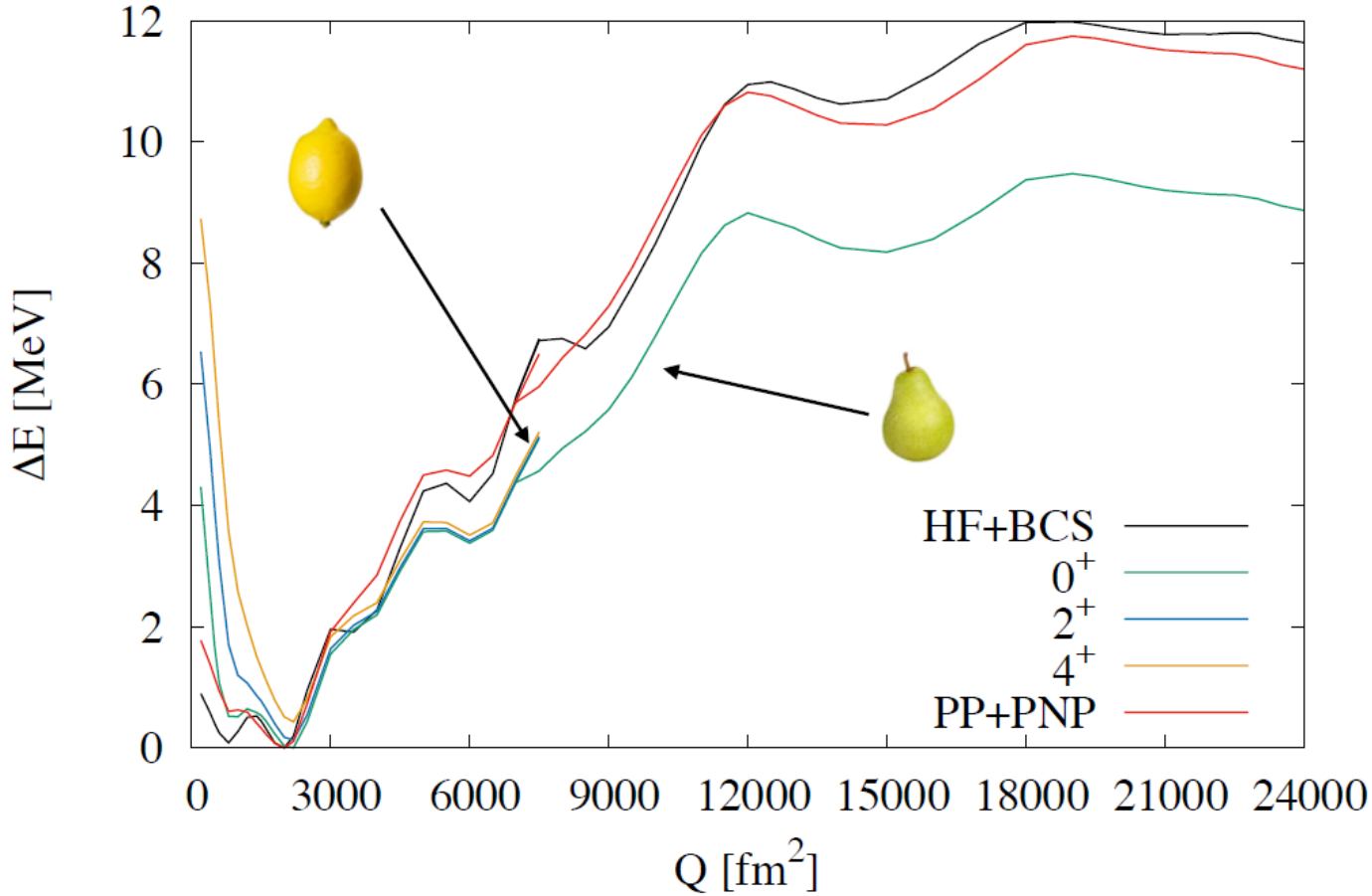
- First aim: asymmetric fission of ^{180}Hg
- Toy test : ^{20}Ne

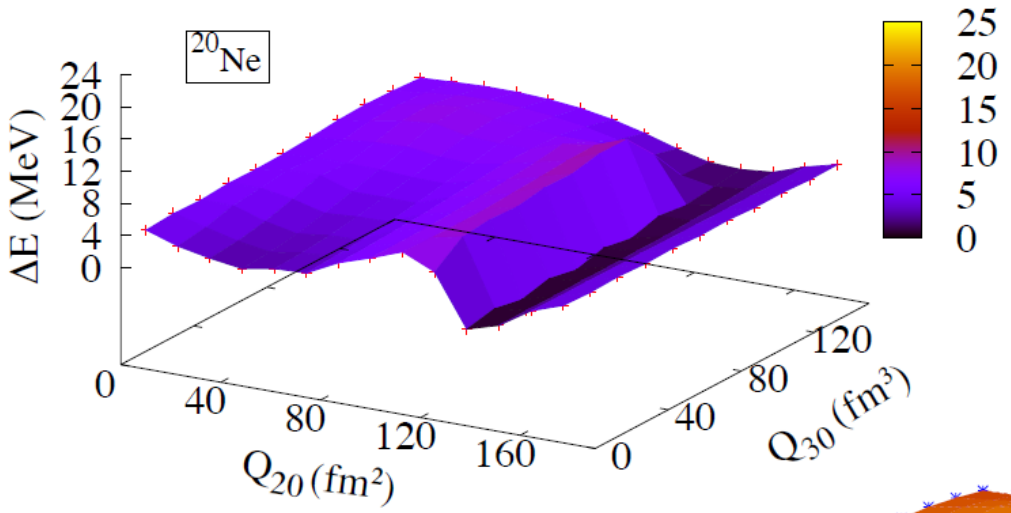
^{180}Hg



- Lower a_s - improved results

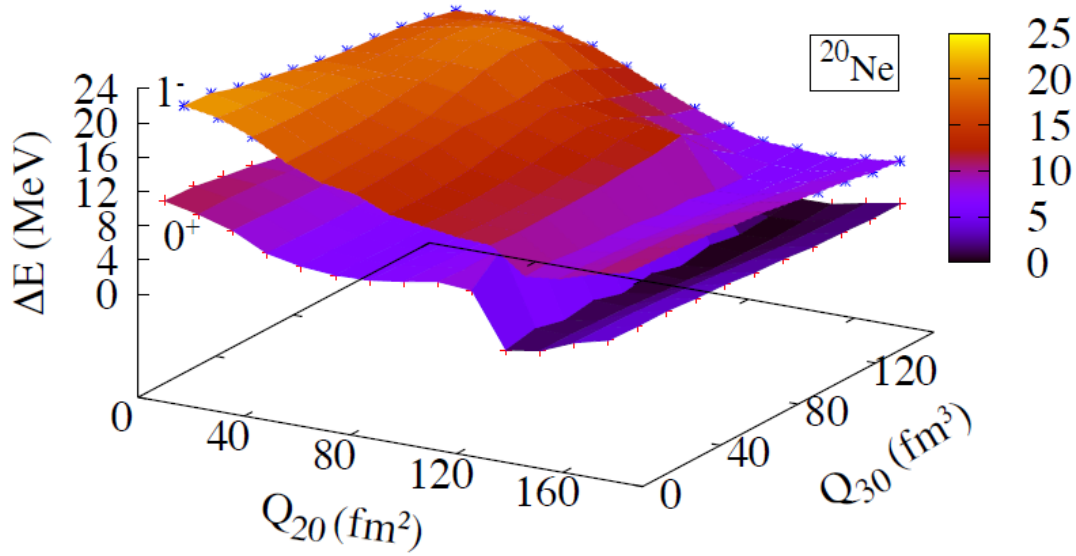
^{180}Hg Calculation for SLy5s1

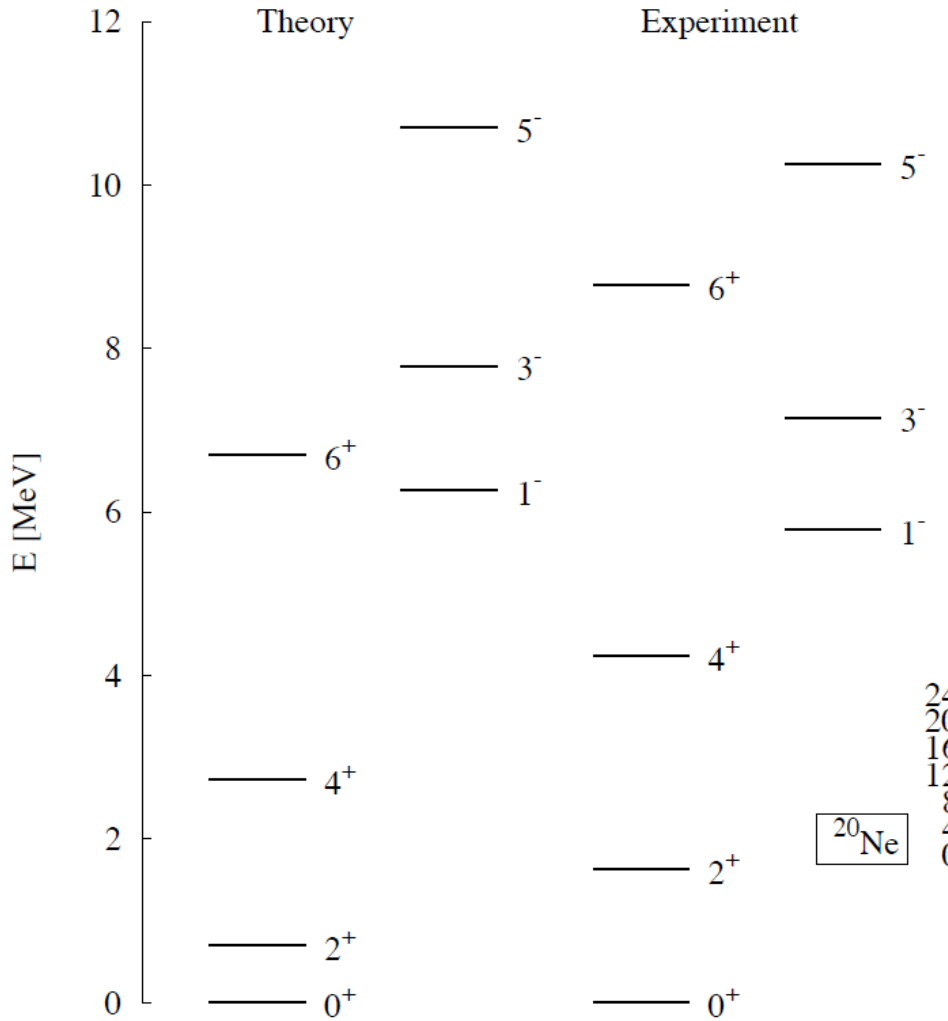




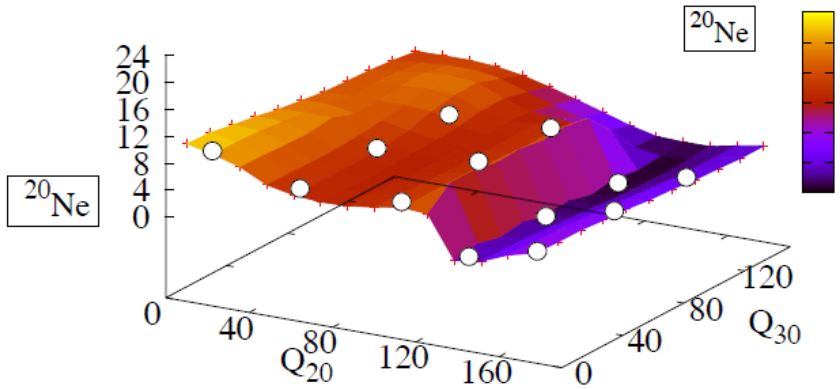
- no pairing, only HF
- SLy5 Skyrme interaction

- Octupole deformed minimum after PP+ +AMP projection





- Configuration mixing after parity and J-projection
- Q_{20} and Q_{30} degrees of freedom



Some final comments

- It works!
- Computing times are high but slowly improving. Today applications feasible up to mass 80 or 100
- We have to learn how to perform the calculations, too many points, analysis is far from trivial
- Excellent framework to study the properties of qp excitations, of cranking states, …
- Main problem is probably the nuclear interaction, still has to be improved