Towards symmetry-unrestricted Skyrme-HFB: MOCCa and its applications.

W. Ryssens[1], M. Bender[1] and P.-H. Heenen [2].

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7th of November 2017

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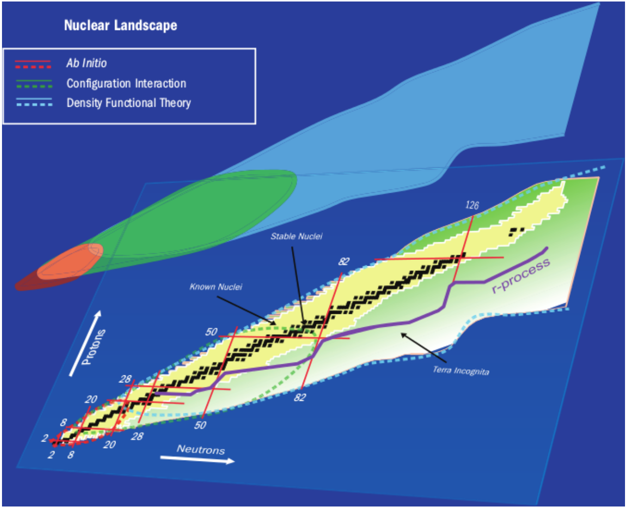
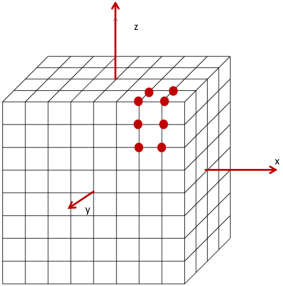
Nuclear energy density functionals



(Outdated) Figure of the UNEDF project from G .F. Bertsch et al., SciDAC Review 6, 48 (2007).



D. Baye *et al.* J. Phys. A **19** (1986).
W.R. *et al.* PRC **92**, 064318 (2015).

Why a coordinate mesh?

- Easily controllable accuracy
  - Number of mesh points
  - Mesh spacing
- Accuracy indepent of shape
  - Important for fission barriers
  - Exponential tail of wavefunction
- Lagrange derivatives
  - High accuracy
  - Variational

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The hero of the story

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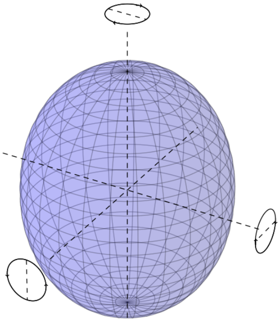
   ,_"""_.
,-|`-...-'|
((_|       |
 `-\       /
   `.___.'
   MOCCa
```

- Generalization of a collection of codes with a long history
  - EV8, EV4, CR8, . . .
- Skyrme Density Functionals
  - SLy5s1 today
- 3D coordinate representation
- Discrete symmetry breaking
  - 16 different combinations
- Pairing: Full HFB
  - For every symmetry combination
  - Non-trivial for signature breaking
- Easy and fast
  - Automatic constraints
  - Better optimization algorithm
  - Automatic blocking identification

Discrete symmetries: $\mathcal{D}_{2h}^{T(D)}$ for nuclei

Single-particle symmetry operators

$$\hat{P}, \hat{R}_{x/y/z}, \check{T}$$



Discrete symmetries: $\mathcal{D}_{2h}^{T(D)}$ for nuclei

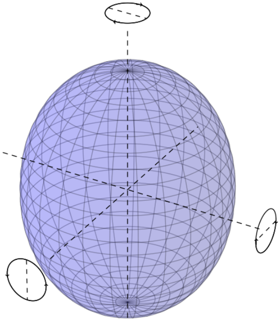
Single-particle symmetry operators

$$\hat{P}, \hat{R}_{x/y/z}, \check{T}$$

give rise to many-body groups

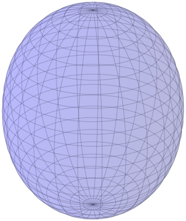
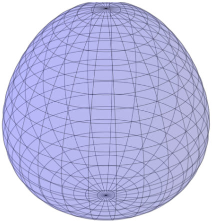
$$\mathcal{D}_{2h}^{T} = \left\{ \hat{1}, \hat{\mathcal{P}}, \check{\mathcal{T}}, \check{\mathcal{P}}^{T}, \hat{\mathcal{R}}_{\mu}, \check{\mathcal{R}}_{\mu}^{T}, \hat{\mathcal{S}}_{\mu}, \check{\mathcal{S}}_{\mu}^{T} \right\} \text{ (even)}$$

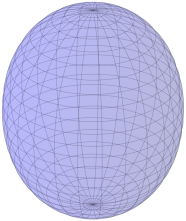
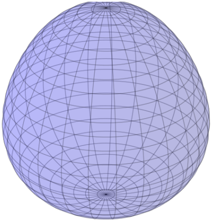
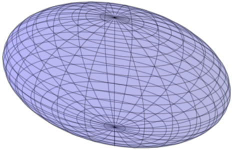
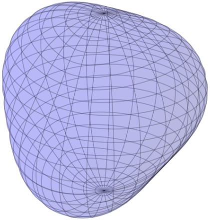
$$\mathcal{D}_{2h}^{TD} = \left\{ \hat{1}, -\hat{1}, \hat{\mathcal{P}}, -\hat{\mathcal{P}}, \check{\mathcal{T}}, -\check{\mathcal{T}}, \hat{\mathcal{R}}_{\mu}, -\hat{\mathcal{R}}_{\mu}, \check{\mathcal{R}}_{\mu}^{T}, -\check{\mathcal{R}}_{\mu}^{T}, \hat{\mathcal{S}}_{\mu}, -\hat{\mathcal{S}}_{\mu}, \check{\mathcal{S}}_{\mu}^{T}, -\check{\mathcal{S}}_{\mu}^{T}, \check{\mathcal{P}}^{T}, -\check{\mathcal{P}}^{T} \right\} \text{ (odd)}$$



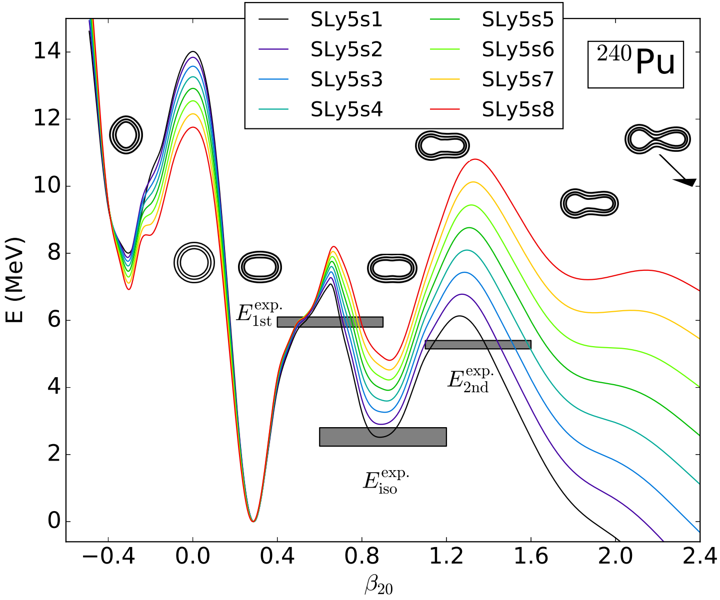
A priori, all subgroups contain different correlations/physics.
Currently, 16 in MOCCa.

Symmetries dictate shapes.

Reflection	Symmetric	Asymmetric
Axial		

Reflection	Symmetric	Asymmetric
Axial		
Non-axial		

Example: Fission barriers



Modelling rotation with Skyrme-HFB cranking Routhian.

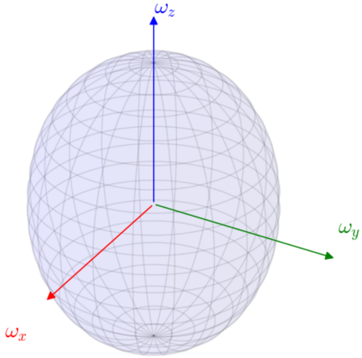
$$R = E - \omega_x\langle\hat{J}_x\rangle - \omega_y\langle\hat{J}_y\rangle - \omega_z\langle\hat{J}_z\rangle$$

Preferred directions ⇒ ~~signatures~~

Compared to experiment

$$\omega(J) = \frac{E(J+1) - E(J-1)}{I(J+1) - I(J-1)} .$$

$$I(J) = \sqrt{J^2 - J^2_{\mathrm{sp}}}$$



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Assume

- **HF basis** of dimension **N**
- h diagonal in this basis

Bogoliubov transformation from particles to quasiparticles

$$\text{Dimension 2N} \left\{ \begin{pmatrix} \hat{\beta} \\ \hat{\beta}^\dagger \end{pmatrix} \right. = \begin{pmatrix} U^\dagger & V^\dagger \\ V^T & U^T \end{pmatrix} \begin{pmatrix} \hat{c} \\ \hat{c}^\dagger \end{pmatrix}$$

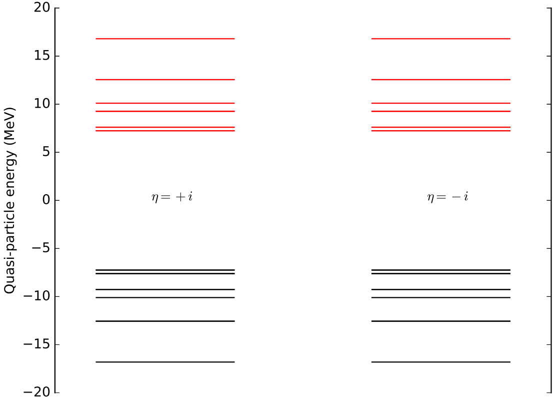
Where the U, V matrices are determined by

$$\mathcal{H} \begin{pmatrix} U \\ V \end{pmatrix} = \underbrace{\begin{pmatrix} h & \Delta \\ -\Delta & -h \end{pmatrix}}_{\text{Dimension 2N}} \begin{pmatrix} U \\ V \end{pmatrix} = E^{qp} \begin{pmatrix} U \\ V \end{pmatrix} .$$

Inherent HFB symmetry: multiple vacua

Inherent symmetry:

$$
\begin{array}{ccc}
U_l & \leftrightarrow & V_l^* \\
V_l & \leftrightarrow & U_l^* \\
E_l^{qp} & \leftrightarrow & -E_l^{qp} \\
\hat{\beta}_l & \leftrightarrow & \hat{\beta}_l^\dagger
\end{array}
$$



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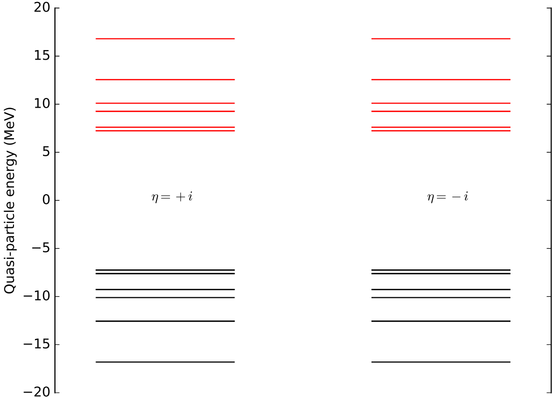
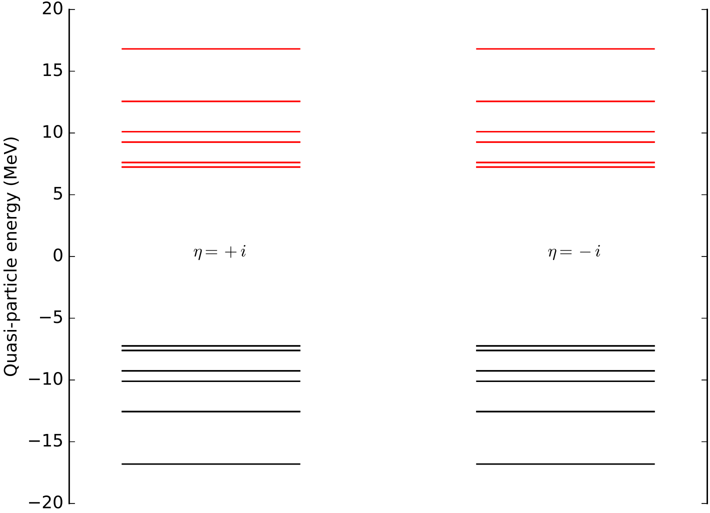


Antilinear, hermitian symmetries come to the rescue.

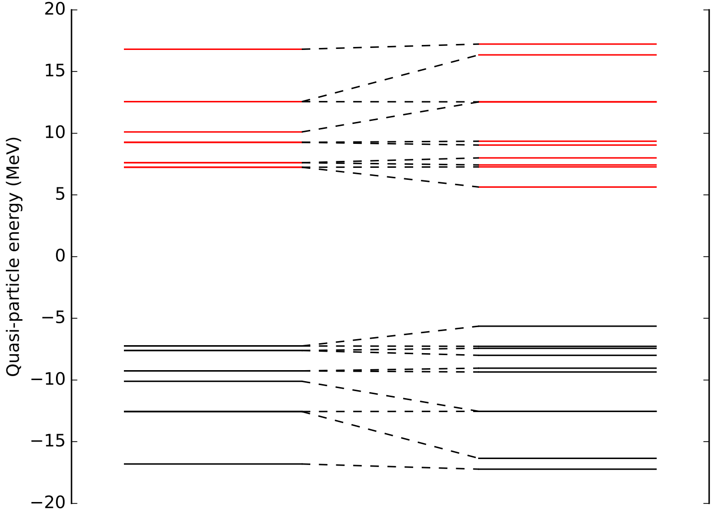
$$\hat{\mathcal{R}}_{x/y/z}, \hat{\mathcal{S}}_{x/y/z}$$

Choosing a vacuum

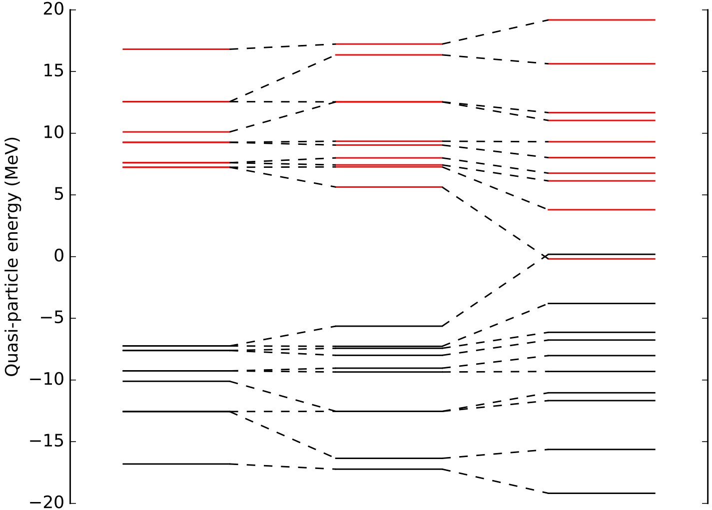
Time-reversal invariant



Lifting the degeneracy



Crossings



Consequences of choosing wrong

$|\Psi_1\rangle$ $\qquad\qquad$ $|\Psi_2\rangle = \hat{\beta}_1^\dagger |\Psi_1\rangle$

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Unwanted one-qp excitation

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Unwanted one-qp excitation

Disaster for any numerical solver.

Problem: Choosing is impossible without antihermitian symmetry.

Signature broken HFB: gradient solver

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Solution: Avoid making a choice.

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Using Thouless ansatz:

$$|\Psi(Z)\rangle = \left[-\frac{1}{2}\sum_{ij} Z_{ij}\beta_i^\dagger \beta_j^\dagger\right] |\Psi_{\text{sym}}\rangle \, . \qquad E(Z, \Psi_0) = \frac{\langle \Psi(Z)|\hat{\mathcal{H}}_{\text{HFB}}|\Psi(Z)\rangle}{\langle \Psi(Z)|\Psi(Z)\rangle} \, .$$

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Minimizing the energy with respect to Z_{ij} gives rise to an iterative scheme

$$\begin{aligned} U^{(\mathrm{iter}+1)} &= U^{(\mathrm{iter})} - \alpha V^{*,(\mathrm{iter})} \left(\mathcal{H}^{20}_{\mathrm{HFB}} - \lambda \mathcal{N}^{20} \right)^* \,, \\ V^{(\mathrm{iter}+1)} &= V^{(\mathrm{iter})} - \alpha U^{*,(\mathrm{iter})} \left(\mathcal{H}^{20}_{\mathrm{HFB}} - \lambda \mathcal{N}^{20} \right)^* \,. \end{aligned}$$

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Form of Thouless ansatz does not allow for unwanted one-qp excitations.

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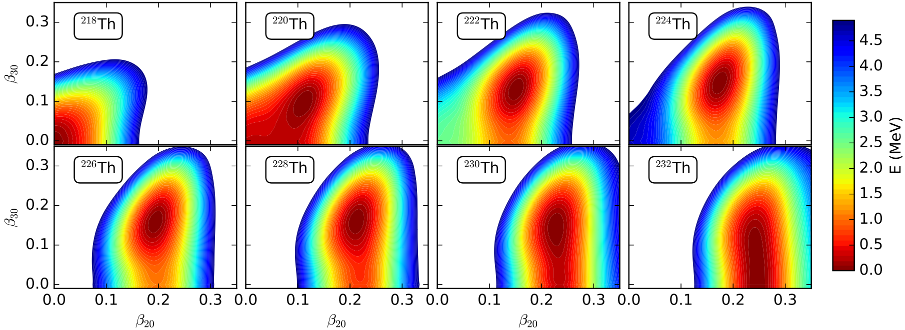
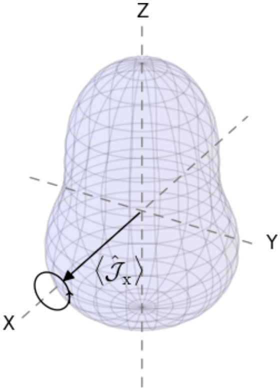
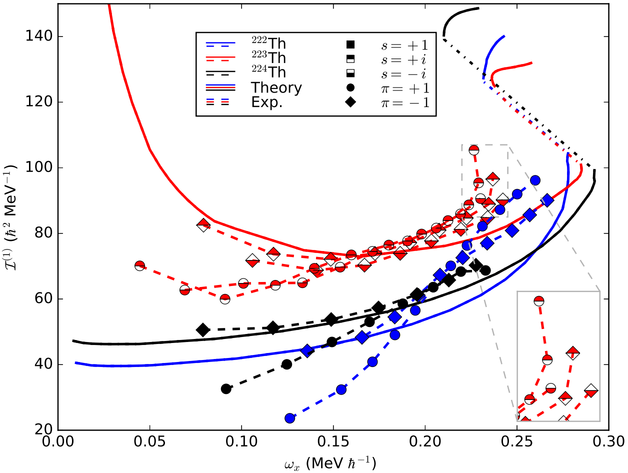
Thorium isotopes with SLy5s1: a function of N



Octupole deformation as function of spin

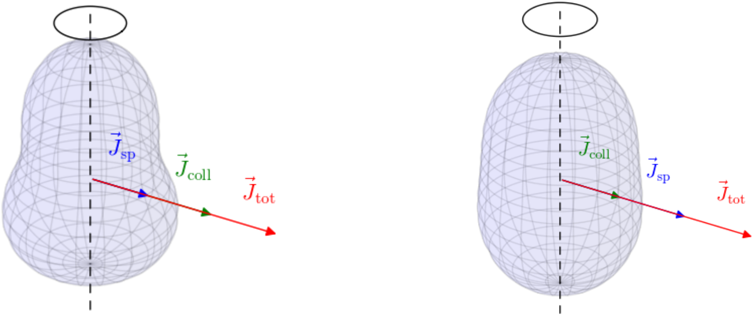


Symmetry	Broken Q.N.	Freedom
Rotations	J	$\beta_{20} \neq 0$
Parity $\hat{P}$	π	$\beta_{30} \neq 0$
Axial rotations	K	$\langle \hat{J}_x \rangle \neq 0$
Time-reversal	N.A.	$\langle \hat{J}_x \rangle \neq 0$
	N.A.	odd neutron
Signature $\hat{R}_x$	η_x	$\beta_{30} \neq 0$



Data from
G. Maquart *et al.*, Phys. Rev. C **95**, 034304 (2017),
J.F. Smith *et al.*, Phys. Rev. Lett. 75, 1050-1053 (1995).

Sudden rearrangement



Intimately related to $(\nu, \pi) = (j15/2, i13/2)$ intruder orbitals.

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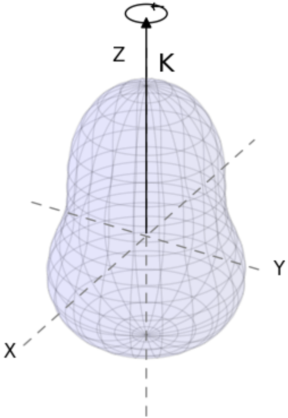
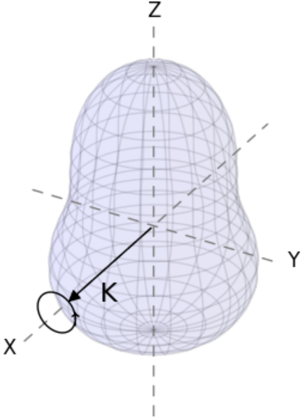
In odd nuclei: ^{223}Th

$$\Delta E = 18 \text{ keV (!)}$$

Signature, axial



No signature, non-axial



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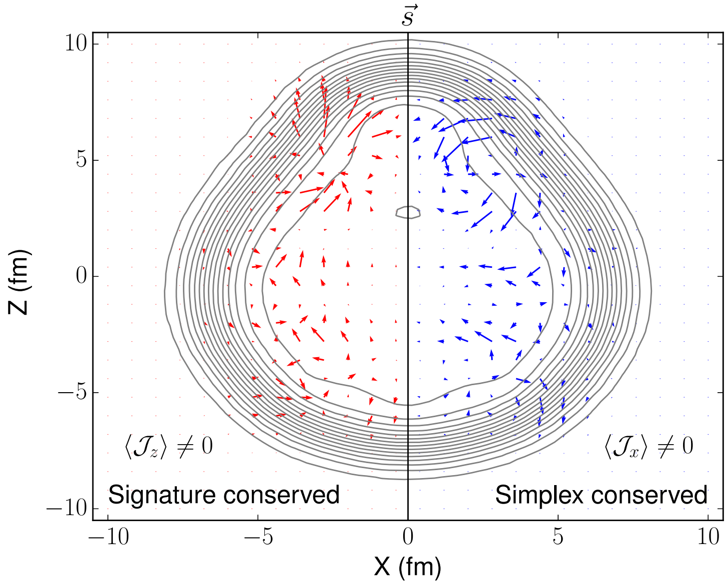
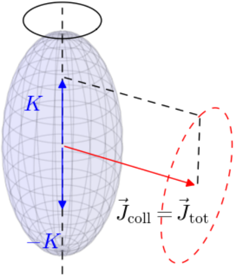
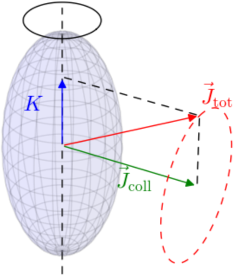


Rotational bands

With signature along rotational axis
Odd particle is allowed to

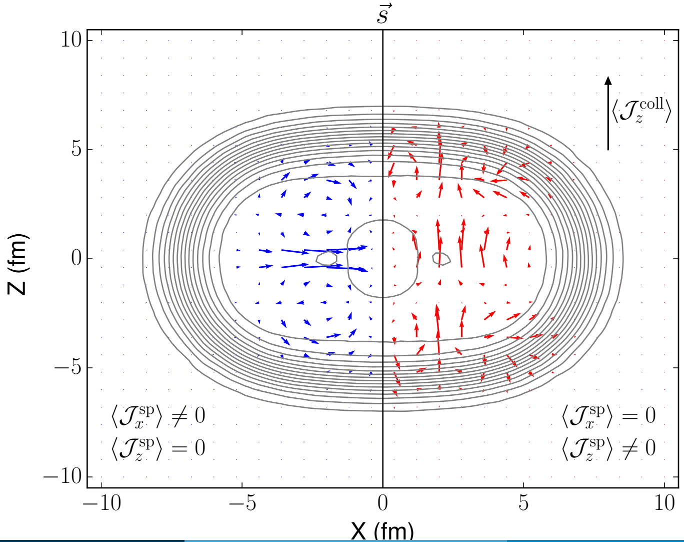


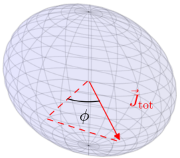
No signature

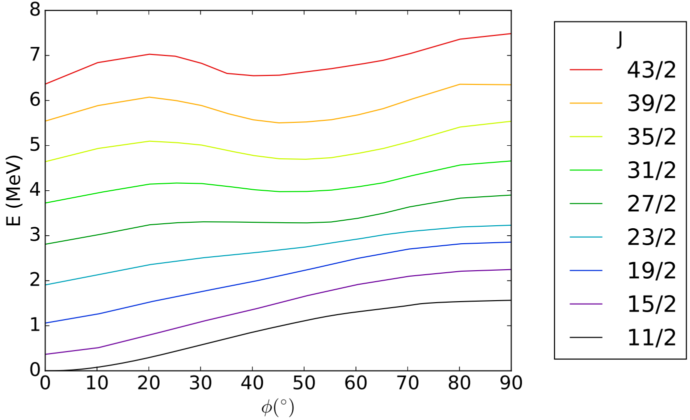


In even-even nuclei: ^{178}Hf

2 quasi-neutron excitations, corresponding to 8^- isomer.




$\vec{J}_{\text{tot}}$
ϕ


E (MeV)
$\phi(^\circ)$
0
1
2
3
4
5
6
7
8
0
10
20
30
40
50
60
70
80
90
J
43/2
39/2
35/2
31/2
27/2
23/2
19/2
15/2
11/2

Many open questions in this regard

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Conclusion

MOCCa

- Intrinsic symmetry breaking is essential.
- Many unexplored correlations are still out there.
- Tool of choice to explore these degrees of freedom.
- Technically advanced and versatile.

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- Ubiquitous when time-reversal is broken.
- Very different spin densities and currents.
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We are working on

- Applying and understanding all the new possibilities.
- Improving existing functionals

Thank you!

Collaborators

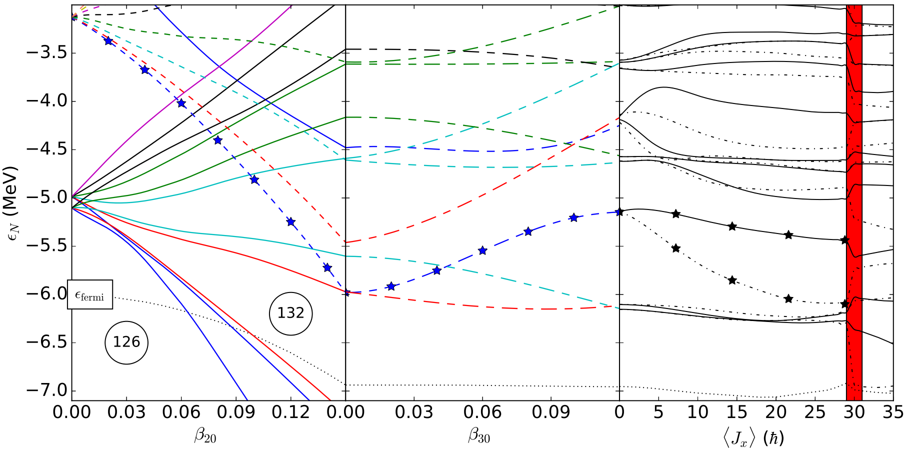
- M. Bender, CNRS
- P.-H. Heenen, ULB

But also

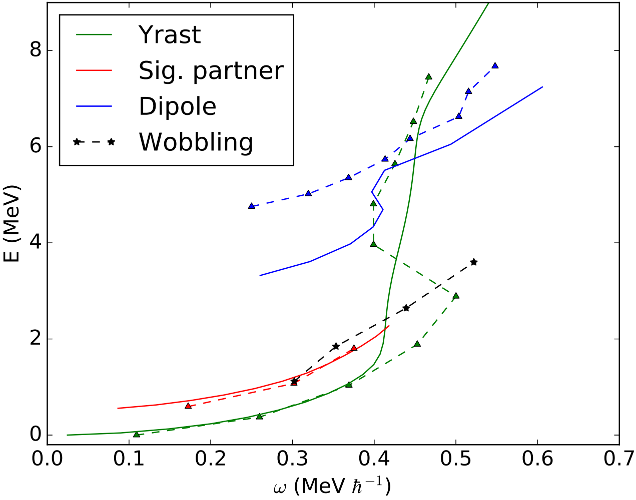
- CC of the IN2P3, French computing resources.
- CECI, Belgian computing resources.
- You, for your attention.

Lyon 1

Neutron nilsson diagram of ^{222}Th



Bands in ^{135}Pr



Exp. data from
PRL **114**, 082501 (2015).