Symmetries and their impact on angular momentum in EDF approaches

As illustrated with a set of Th isotopes.

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Abstract

With the advent of tracking-gamma-ray spectroscopy, a wealth of rich experimental on **exotic nuclei** at **high spin** has become available in recent years. Within a **mean-field** context, such structures are usually related to nuclear configurations that break **intrinsic symmetries**: a configuration with non-zero **octupole** deformation is no longer reflection symmetric for instance. I will discuss the ongoing effort in Lyon and Brussels to extend the applicability of existing energy density functional approaches to describe **rotational bands** based on various **symmetry-breaking** configurations, including **odd-mass** nuclei. Applications to rotational bands in octupole deformed nuclei and so-called ~~'wobbling' bands~~ will be presented, and a particular attention will be devoted to the role played by various **degrees of freedom of the angular momentum**.

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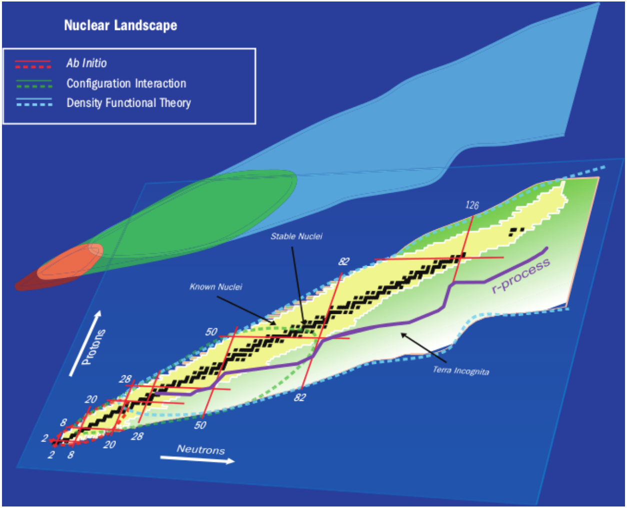

(Outdated) Figure of the UNEDF project from G .F. Bertsch et al., SciDAC Review 6, 48 (2007).

EDF optimization

Find the **minimum** of $E(\rho, \tau, J_{\mu\nu})$ in a given **variational** space

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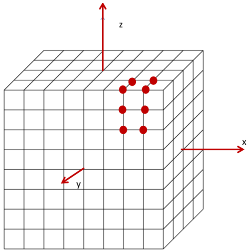
Variational space

- Single-particle states form ...
- ... Many-body states as (generalized) product states
- Represented on a 3D mesh
- Also determined by **symmetries** !



Find the **minimum** of $E(\rho, \tau, J_{\mu\nu})$ in a given **variational** space

Variational space

- Single-particle states form . . .
- . . . Many-body states as (generalized) product states
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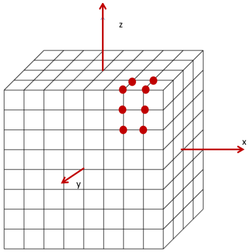
Products states maintain simplicity, . . .
Symmetry breaking to enrich!



Self-consistent EDF calculations

$\boxed{\Psi_{\text{many-body}} = \text{Product wavefunction}}$

Self-consistent EDF calculations

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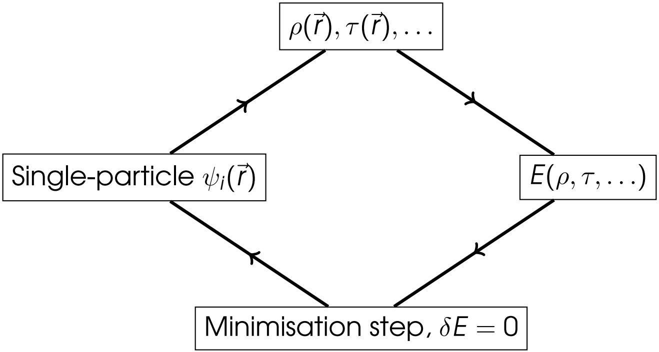

Self-consistent EDF calculations

$\Psi_{\text{many-body}}$ = Product wavefunction

$$\begin{tikzcd}
 & \boxed{\rho(\vec{r}), \tau(\vec{r}), \ldots} \arrow[dr] & \\
\boxed{\text{Single-particle } \psi_i(\vec{r})} \arrow[ur] & & \boxed{E(\rho, \tau, \ldots)} \arrow[dl] \\
 & \boxed{\text{Minimisation step, } \delta E = 0} \arrow[ul] &
\end{tikzcd}$$

Symmetries and quantum numbers of $\psi_i \Rightarrow$ simplification
Complexity determined by the single-particle space

Multiple terms

$$E_{\text{tot}} = E_{\text{kin}} + E_{\text{Skyrme}} + E_{\text{Coul}} + E_{\text{cm}} + E_{\text{pair}} \, ,$$

The more or less standard Skyrme part is the following

$$E_{\text{Skyrme}} = \sum_{t=0,1} \int d^3 r \Big[C_t^{\rho} \, \rho_t^2(\vec{r}) + C_t^{\rho^{\alpha}} \, \rho_0^{\alpha}(\vec{r}) \, \rho_t^2(\vec{r}) + C_t^{\tau} \, \rho_t(\vec{r}) \, \tau_t(\vec{r})$$
$$+ C_t^{\Delta\rho} \, \rho_t(\vec{r}) \, \Delta\rho_t(\vec{r}) + C_t^{\nabla\cdot J} \rho_t(\vec{r}) \, \nabla \cdot \vec{J}_t(\vec{r}) - C_t^{T} \sum_{\mu,\nu} J_{t,\mu\nu}(\vec{r}) \, J_{t,\mu\nu}(\vec{r}) \Big] \, .$$

which has

- Densities: $\rho, \tau, J_{\mu\nu}$
- $\sim$ **10** parameters . . .
- . . . fitted to a few masses and radii.

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Easy to calculate!

Skyrme (NLO) functional

Multiple terms

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which has

- Densities: $\rho, \tau, J_{\mu\nu}$
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Easy to calculate!

Only half of the story; also time-odd terms!

What we try to reach

Global microscopic framework to describe

Bulk properties

- Masses
- Radii

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Low-energy spectroscopy

- Ground states
  - 0^+ for even-even nuclei
  - J^π for even-odd
  - ~~odd-odd~~
- Low-lying excitations
  - Isomers of various kinds
  - Rotational bands

What we try to reach

Global microscopic framework to describe

Bulk properties

- Masses
- Radii

Low-energy spectroscopy

- Ground states
  - 0^+ for even-even nuclei
  - J^π for even-odd
  - ~~odd-odd~~
- Low-lying excitations
  - Isomers of various kinds
  - Rotational bands

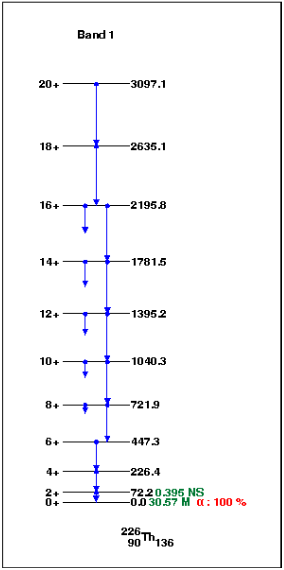
Rather good: **HFB17** describes

S.Goriely et al., PRL **102**, 152503 (2009).

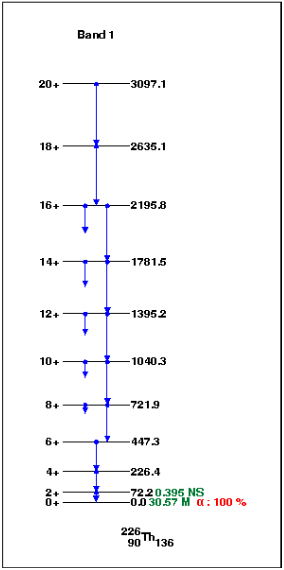
- **2149** masses
  RMS deviation = **0.581** MeV
- **792** charge radii
  RMS deviation = **0.0313** fm

This is not easy at all . . .

Rotational bands



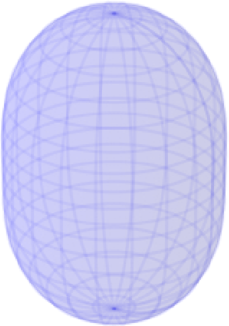
Data for ^{226}Th from NNDC



Data for ^{226}Th from NNDC

Seems very much like the spectrum of a rotator

$$E \sim J(J+1)$$



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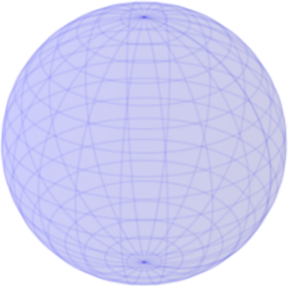
a. Ultra-Fast calculations ($\sim$seconds)
b. Symmetries respected
c. Most EDFs fitted at this level
d. Single-particle quantum numbers J, J_z, π

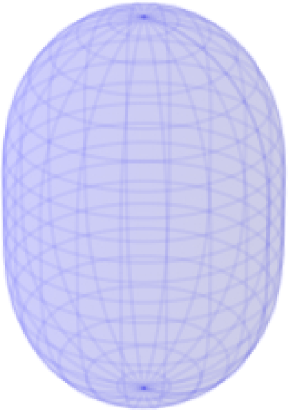


Axial symmetry: Ellipsoids

a Fast calculations ($\sim$minutes)

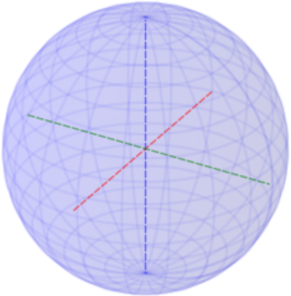
b One symmetry axis

c Single-particle quantum numbers $K = J_z, \pi$



Triaxial shapes

a Slow calculations ($\sim$ hours/days)
b No more continuous symmetries



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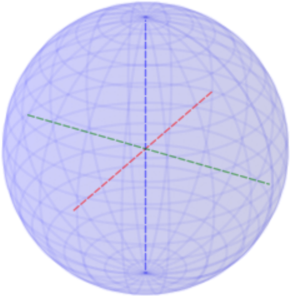

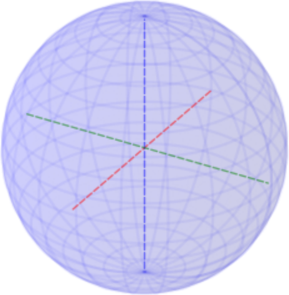

a Slow calculations ($\sim$ hours/days)

b No more continuous symmetries

c Single-particle quantum numbers π

d Several possible discrete symmetries

General group of symmetries for even-even nuclei

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

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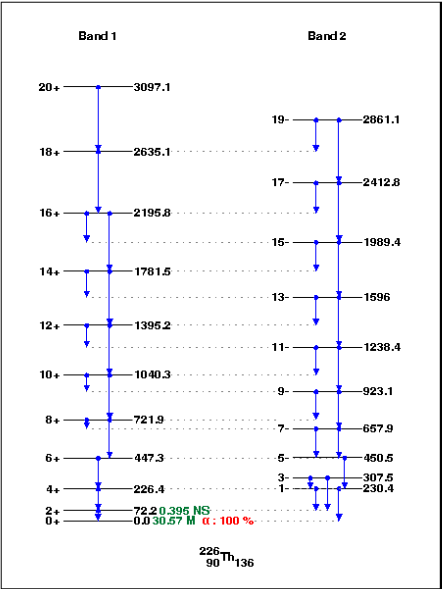
* Skyrme Density Functionals

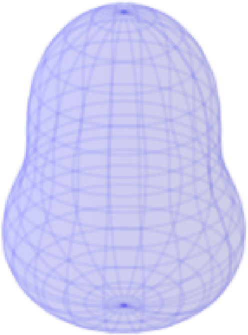
  SLy5s1 today
  (R. Jodon et al. , PRC **94**, 024335 (2016))
* 3D coordinate representation
* Discrete symmetry breaking

  16(!) different combinations
* Generalization of a collection of codes

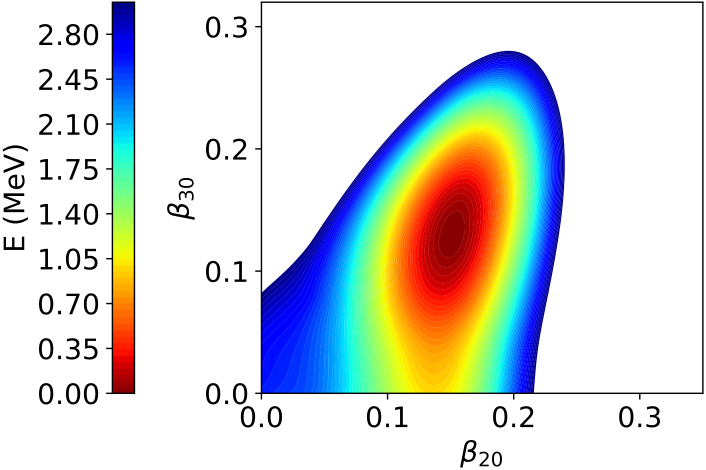
  EV8, EV4, CR8, . . .
* HF, HF+BCS or HFB

  Non-trivial for some symmetries !
* Easy to use and fast


Band 1
Band 2
20+ 3097.1
18+ 2635.1
16+ 2195.8
14+ 1781.5
12+ 1395.2
10+ 1040.3
8+ 721.9
6+ 447.3
4+ 226.4
2+ 72.2 0.395 NS
0+ 0.0 30.57 M α : 100 %
19- 2861.1
17- 2412.8
15- 1989.4
13- 1596
11- 1238.4
9- 923.1
7- 657.9
5- 450.5
3- 307.5
1- 230.4
$^{226}_{90}Th_{136}$

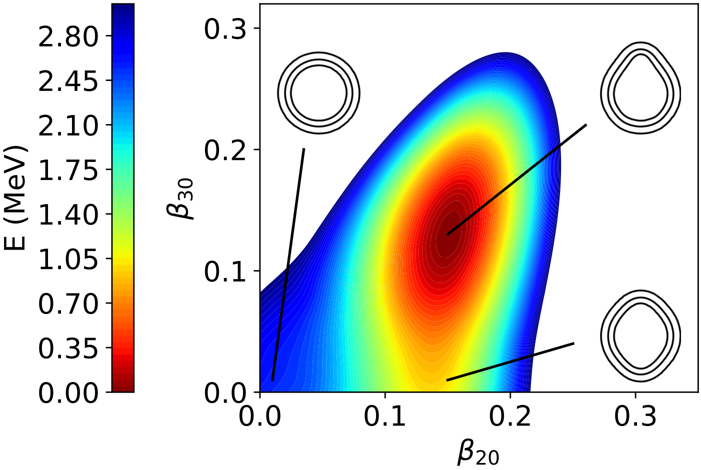


^{222}Th



$$\beta_{\ell m} = \frac{4\pi}{3R_0 A^{1/3+\ell}} \int d^3\vec{r}\, \rho(\vec{r}) r^\ell Y_{\ell m}(\vec{r})$$

^{222}Th



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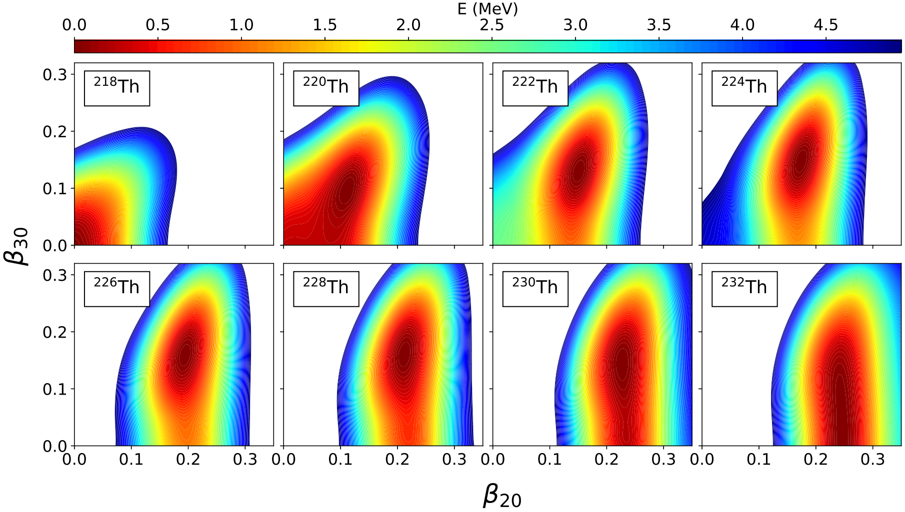
Even-even Thoriums



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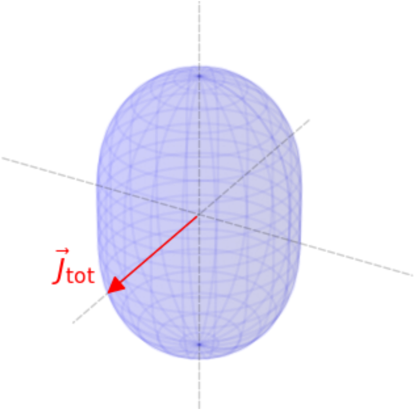
The inclusion of angular momentum



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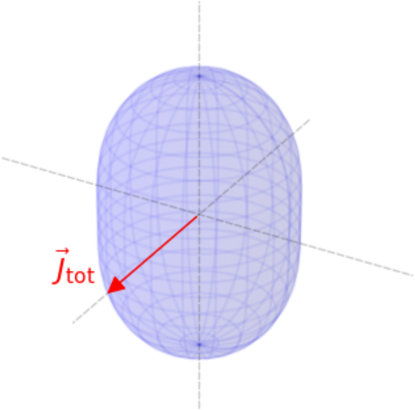
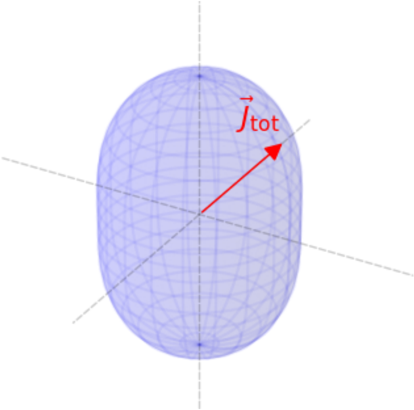
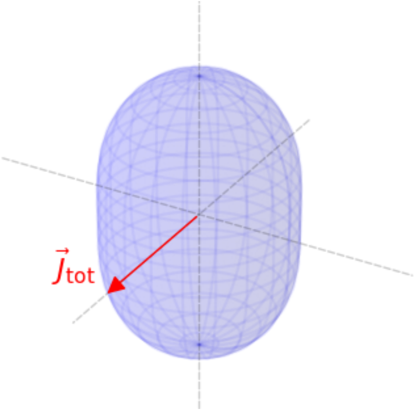


$$\check{\mathcal{T}}$$

$$\Rightarrow$$

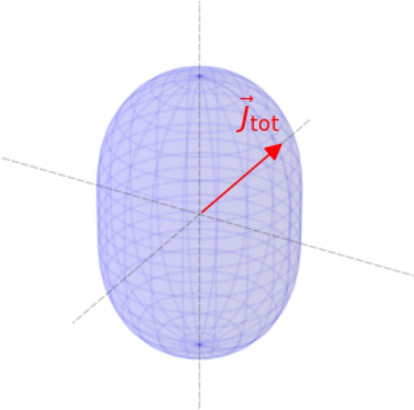




$$\check{\mathcal{T}}$$

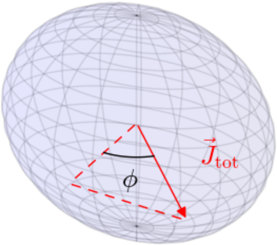
$$\Rightarrow$$

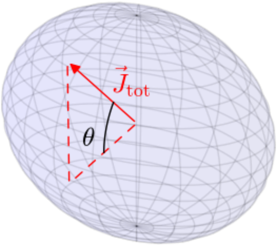
$$\hat{\mathcal{R}}_{y,z}$$



Angular momentum breaks symmetries

Unrestricted angular momentum $\Rightarrow$ no more **rotational** symmetries!





Beyond even-even groundstates

Things you can calculate

1. Even-even nuclei
   (ground states in general)

Beyond even-even groundstates

Things you can calculate

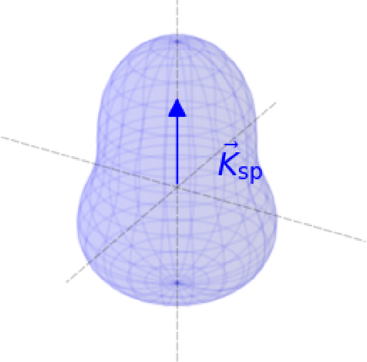
1. Even-even nuclei (ground states in general)

Things you can't calculate

1. Odd nuclei
2. Odd-odd nuclei
3. Rotational bands
4. Non-collective states in even-even nuclei
5. Time-dependent calculations (TDHF)
6. ...

Axial configurations

K quantum number



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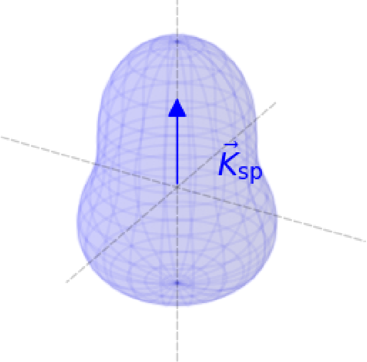
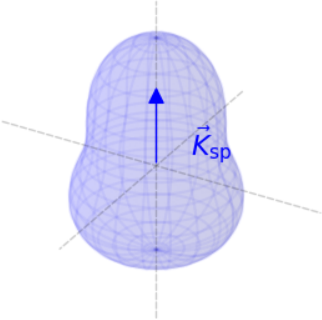
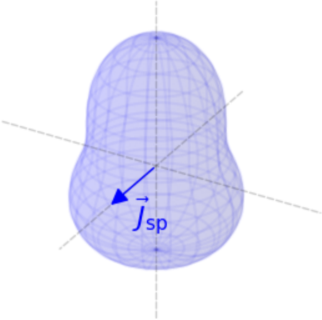


To be compared to experiment

A	Exp.	Th.
221	$7/2^+$	1/2
223	$5/2^+$	5/2
225	$3/2^+$	3/2
227	$1/2^+$	1/2
229	$5/2^+$	1/2
231	$5/2^+$	1/2





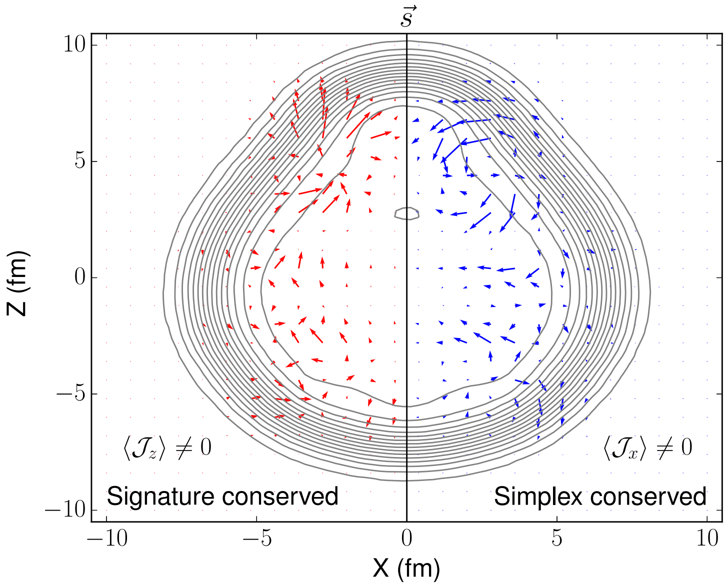
Quantized K

Comparable to experiment

Non quantized $\langle J_x \rangle$

Experiment?

Non-axial configurations



Modelling rotation with
Skyrme-HFB **cranking** Routhian.

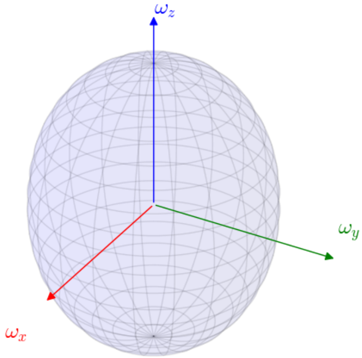
$$R = E - \omega_x\langle\hat{J}_x\rangle - \omega_y\langle\hat{J}_y\rangle - \omega_z\langle\hat{J}_z\rangle \, ,$$

Experimental quantities:

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

$$\mathcal{I}^{(1)}_{\mathrm{exp.}} = \frac{I(J+1)}{\omega(J)}$$

$$\mathcal{I}^{(1)}_{\mathrm{theo.}} = \frac{|\langle\vec{J}\rangle|}{|\omega|} \, .$$



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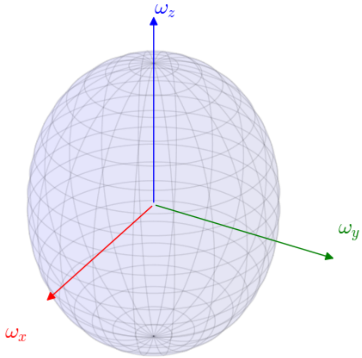
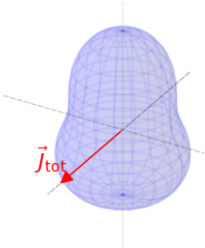
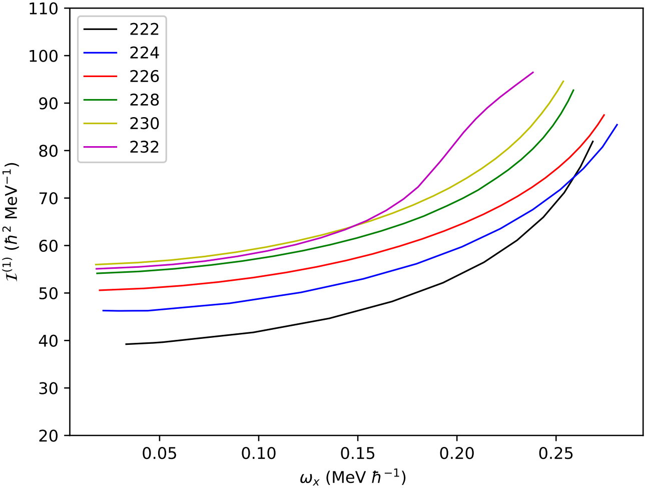
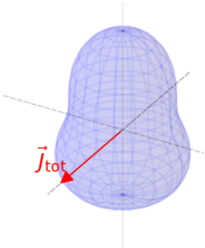
NO control over
collective J vs single-particle J

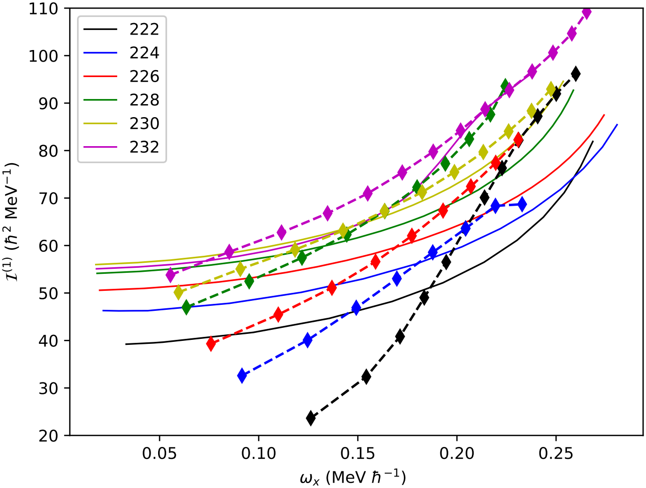






Exp. data from NNDC.



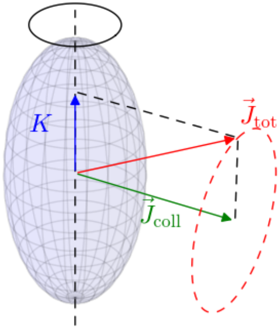


Exp. data from NNDC.

Two sources for angular momentum

a Single-particle

b Collective

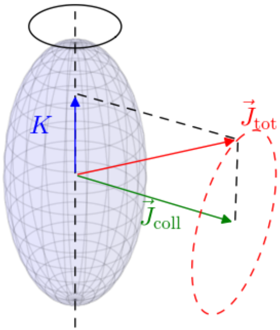


Two sources for angular momentum

a Single-particle

b Collective

Staples of simpler models (particle-rotor)



Two sources for angular momentum

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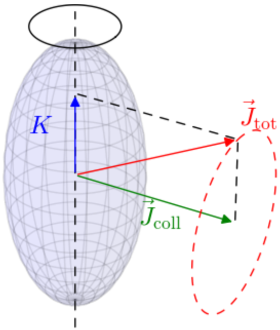
b Collective

Staples of simpler models (particle-rotor)

NOT well-defined
in a self-consistent model



Collective J vs single-particle J

Two sources for angular momentum

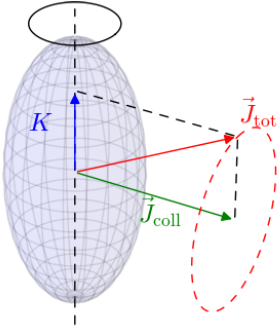
a Single-particle

b Collective

Staples of simpler models (particle-rotor)

NOT well-defined in a self-consistent model

But it seems to be the only way to connect to experiment . . .

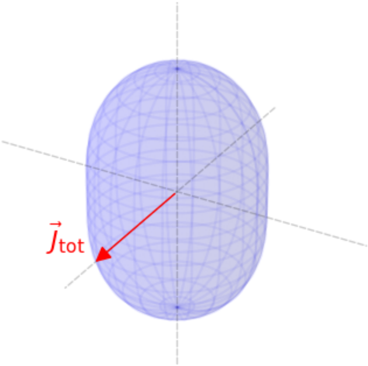


Connecting to experiment $J_{\mathrm{exp.}}$?

Map onto rotational models

Fully collective (even-even)

$$\left|\langle \vec{J} \rangle\right| = \sqrt{J_{\mathrm{exp.}}(J_{\mathrm{exp.}} + 1)}.$$



Connecting to experiment $J_{\mathrm{exp.}}$?

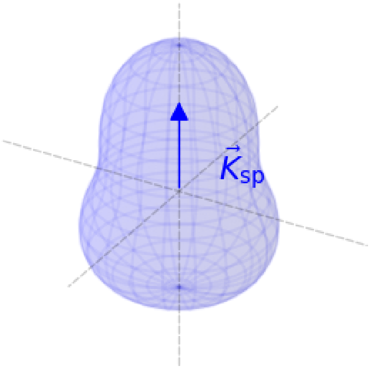
Map onto rotational models

Fully collective (even-even)

$$\left|\langle\vec{J}\rangle\right| = \sqrt{J_{\mathrm{exp.}}(J_{\mathrm{exp.}}+1)}.$$

Fully Single-particle (odd)

$$K = J_{\mathrm{exp.}}$$



Map onto rotational models

Fully collective (even-even)

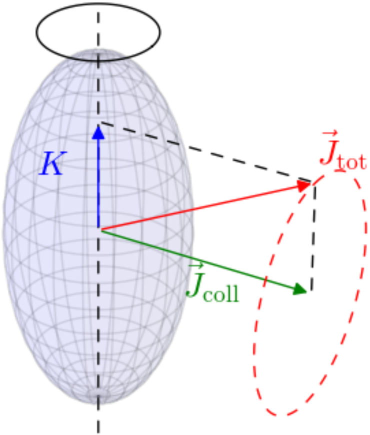
$$\left|\langle\vec{J}\rangle\right| = \sqrt{J_{\text{exp.}}(J_{\text{exp.}}+1)}.$$

Fully Single-particle (odd)

$$K = J_{\text{exp.}}$$

Mixed (strong-coupling)

$$\left|\langle\vec{J}_{\text{coll.}}\rangle\right| = \sqrt{J_{\text{exp.}}(J_{\text{exp.}}+1) - K^2},$$



Connecting to experiment $J_{\text{exp.}}$?

Map onto rotational models

Fully collective (even-even)

$$\left|\langle \vec{J} \rangle\right| = \sqrt{J_{\text{exp.}}(J_{\text{exp.}} + 1)}.$$

Fully Single-particle (odd)

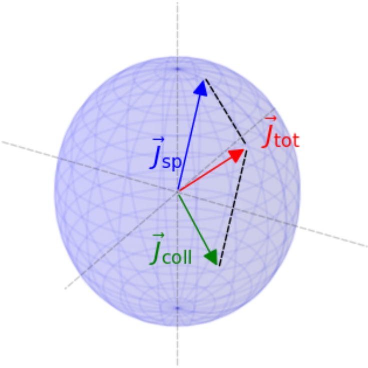
$$K = J_{\text{exp.}}$$

Mixed (strong-coupling)

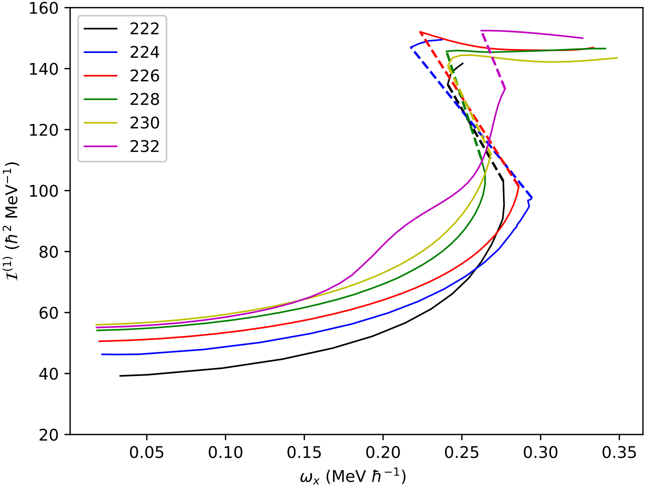
$$\left|\langle \vec{J}_{\text{coll.}} \rangle\right| = \sqrt{J_{\text{exp.}}(J_{\text{exp.}} + 1) - K^2},$$

Mixed, general

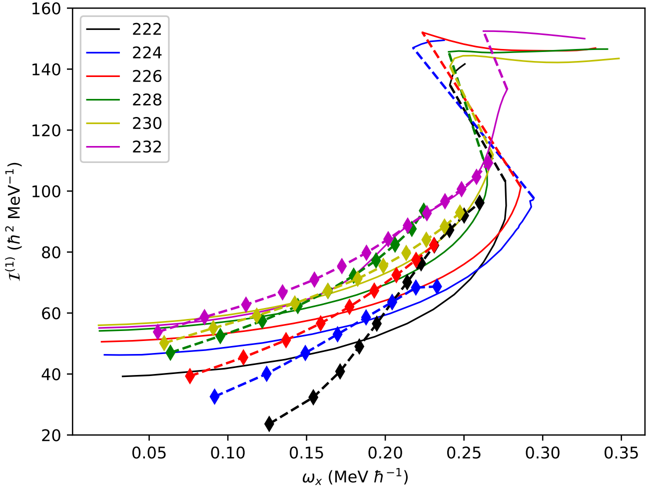
$$\left|\langle \vec{J} \rangle\right| \sim J_{\text{exp}} \qquad ???$$



Moment of inertia at high spin



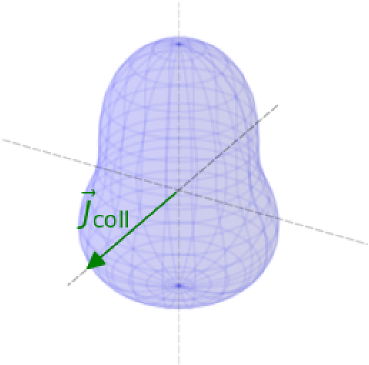
Exp. data from NNDC.



Exp. data from NNDC.

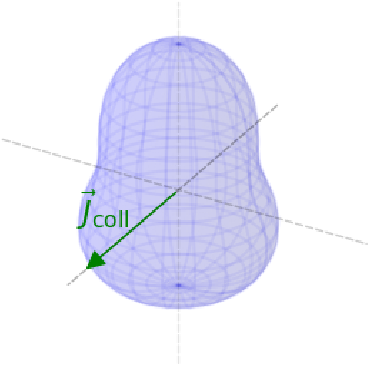
Sudden change of shape

Before

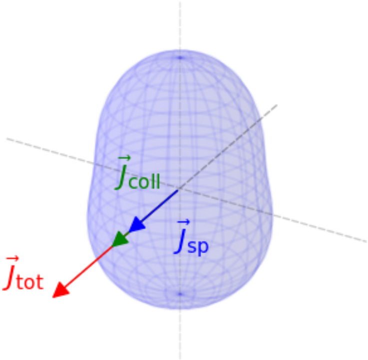


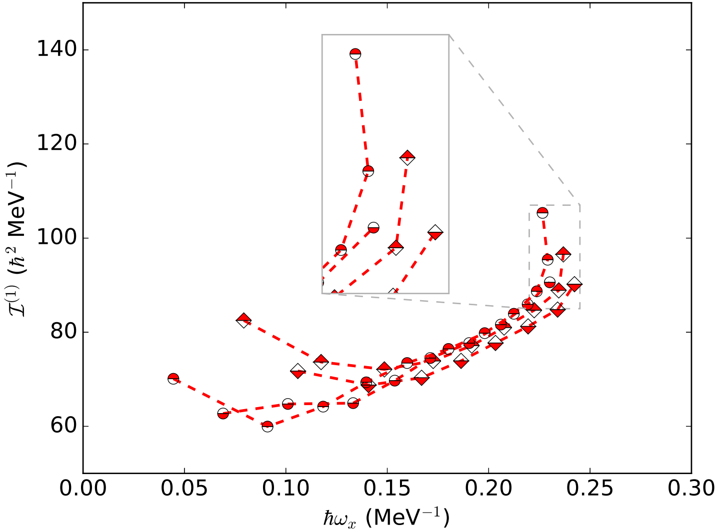
Sudden change of shape

<u>Before</u>

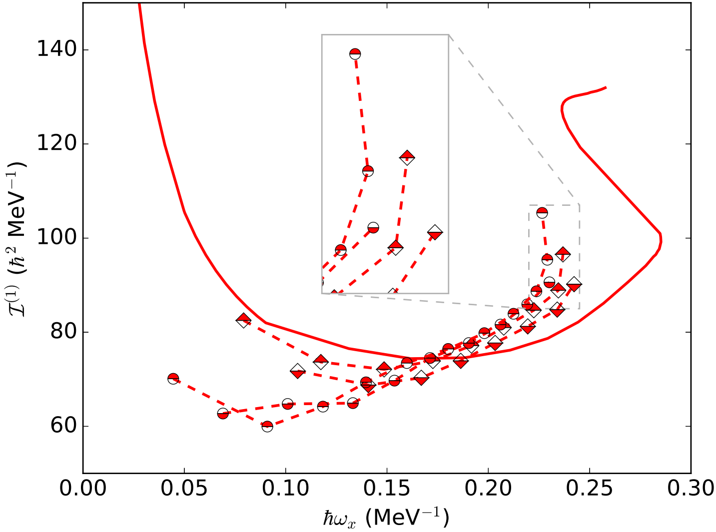


<u>After</u>





Exp. data from G. Maquart et al., PRC **95**, 034304 (2017).



Exp. data from G. Maquart et al., PRC **95**, 034304 (2017).

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- Applicable to ALL nuclei
- Symmetry breaking is key
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- Spectroscopy often problematic . . .

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  Wobbling bands
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Future

- Parameterizations for spectroscopy (SHEET project)
- Parameterizations allowing for symmetry restoration

Thank you!

Collaborators

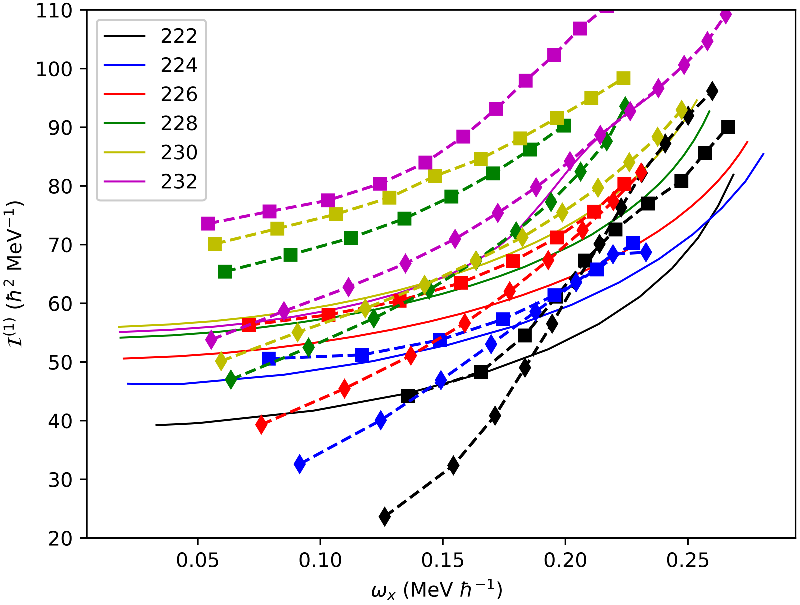
Paul-Henri Heenen	ULB
Michael Bender	IPN Lyon
Benjamin Bally	UA Madrid
Karim Bennaceur	IPN Lyon
Dany Davesne	IPN Lyon
Jacques Meyer	IPN Lyon

No longer active :(

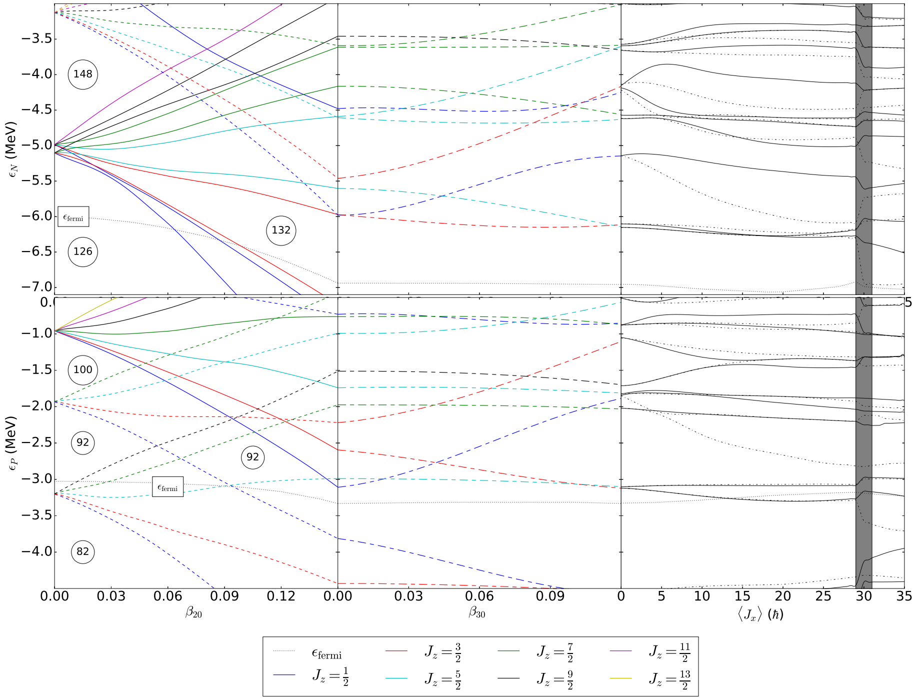
Benoît Avez	Robin Jodon
Veerle Hellemans	Jeremy Sadoudi

Thanks for the support in form of CPU time (for W.R.)

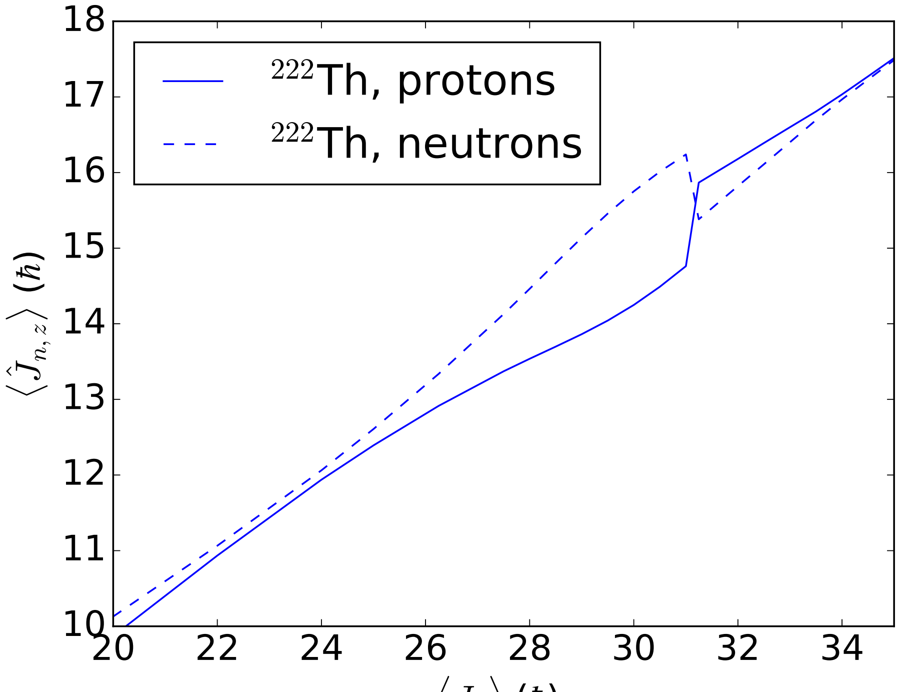
CC of the IN2P3	CNRS, France
CECI network	FNRS, Belgium

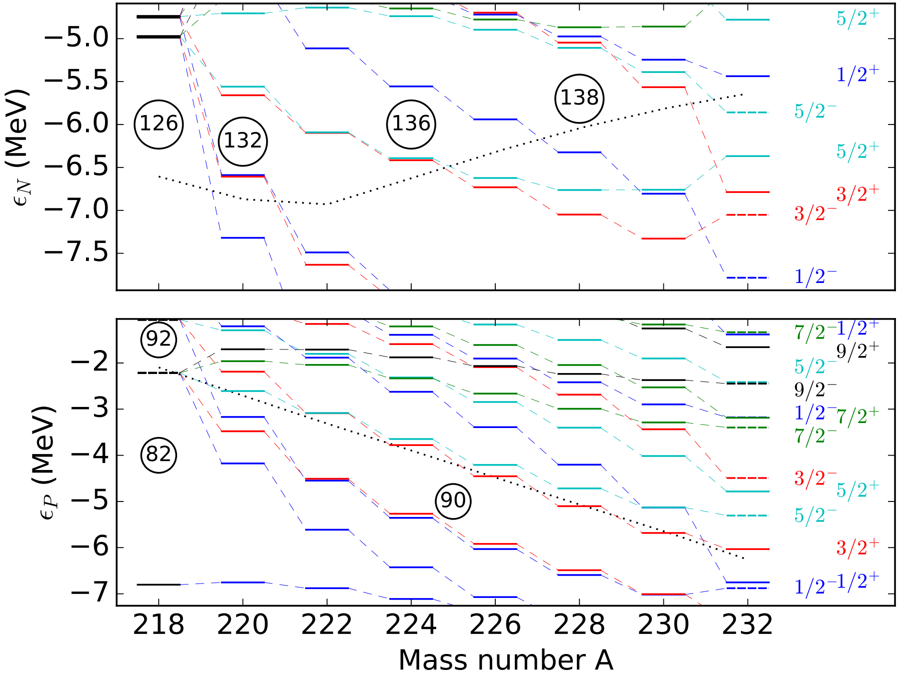


222
224
226
228
230
232
110
100
90
80
70
60
50
40
30
20
0.05
0.10
0.15
0.20
0.25
ω_x (MeV $\hbar^{-1}$)
$\mathcal{I}^{(1)}$ ($\hbar^2$ MeV^{-1})

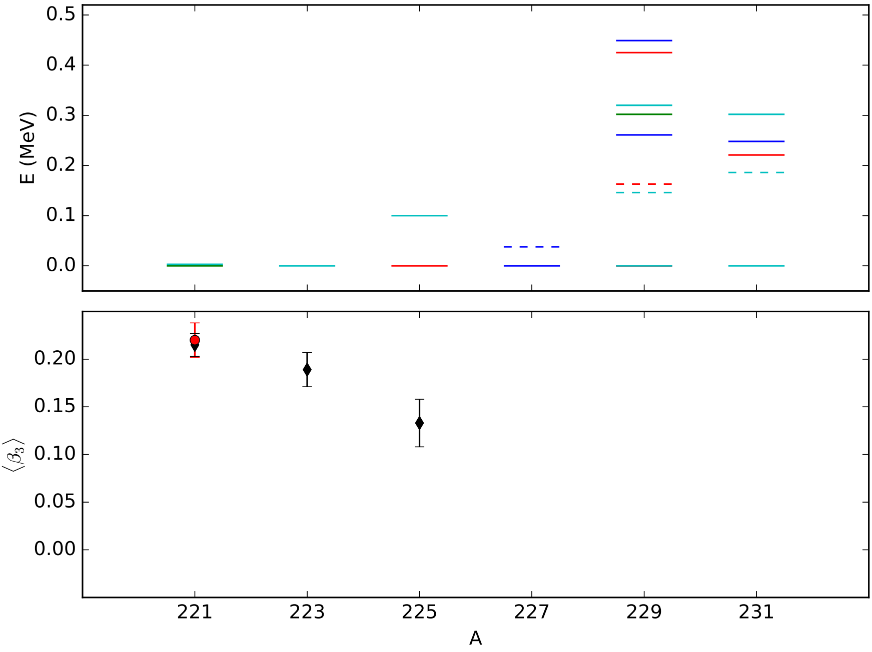


148
126
132
$\epsilon_{\rm fermi}$
100
92
92
82
ϵ_N (MeV)
ϵ_P (MeV)
β_{20}
β_{30}
$\langle J_x \rangle$ ($\hbar$)
$\epsilon_{\rm fermi}$
$J_z = \frac{1}{2}$
$J_z = \frac{3}{2}$
$J_z = \frac{5}{2}$
$J_z = \frac{7}{2}$
$J_z = \frac{9}{2}$
$J_z = \frac{11}{2}$
$J_z = \frac{13}{2}$

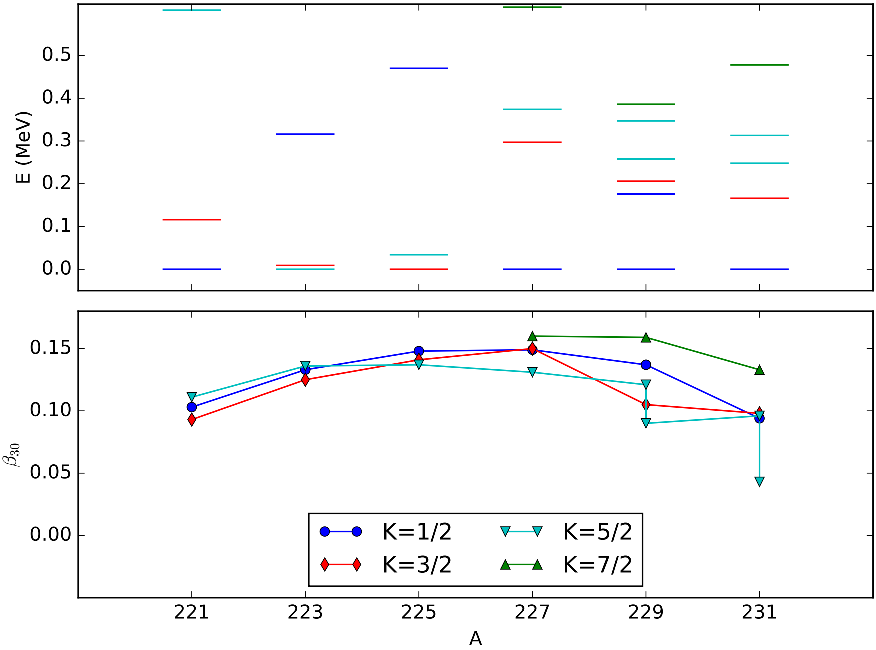

^{222}Th, protons
^{222}Th, neutrons
$\langle \hat{J}_{n,z} \rangle$ ($\hbar$)
18
17
16
15
14
13
12
11
10
20
22
24
26
28
30
32
34



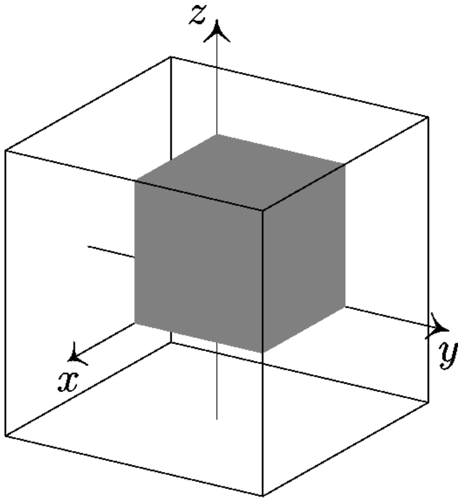
ϵ_N (MeV)
−5.0
−5.5
−6.0
−6.5
−7.0
−7.5
126
132
136
138
$5/2^+$
$1/2^+$
$5/2^-$
$5/2^+$
$3/2^+$
$3/2^-$
$1/2^-$
ϵ_P (MeV)
−2
−3
−4
−5
−6
−7
92
82
90
$7/2^-$ $1/2^+$
$9/2^+$
$5/2^-$
$9/2^-$
$1/2^-$ $7/2^+$
$7/2^-$
$3/2^-$
$5/2^+$
$5/2^-$
$3/2^+$
$1/2^-$ $1/2^+$
218
220
222
224
226
228
230
232
Mass number A



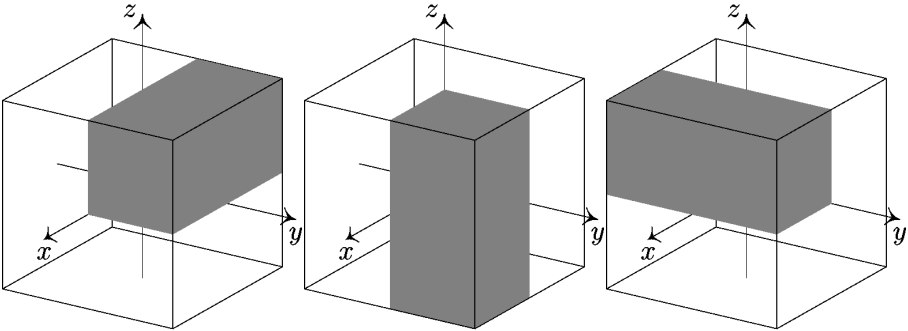
E (MeV)
0.5
0.4
0.3
0.2
0.1
0.0
$\langle \beta_3 \rangle$
0.20
0.15
0.10
0.05
0.00
221
223
225
227
229
231
A


E (MeV)
0.0
0.1
0.2
0.3
0.4
0.5
β_{30}
0.00
0.05
0.10
0.15
K=1/2
K=3/2
K=5/2
K=7/2
221
223
225
227
229
231
A

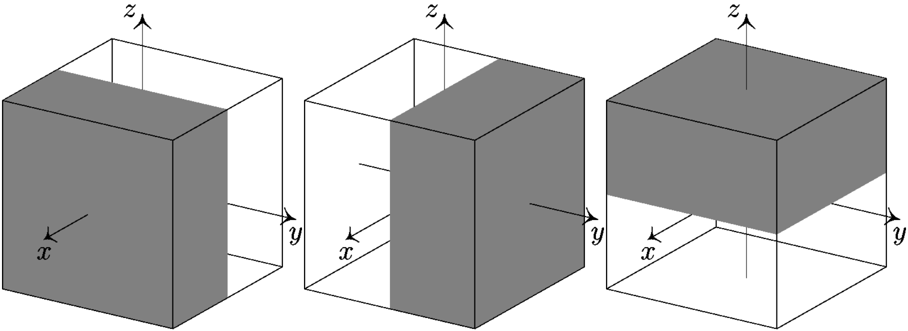
Possibilities

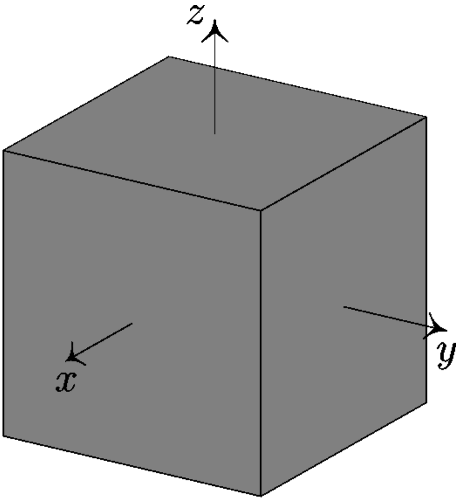


Possibilities

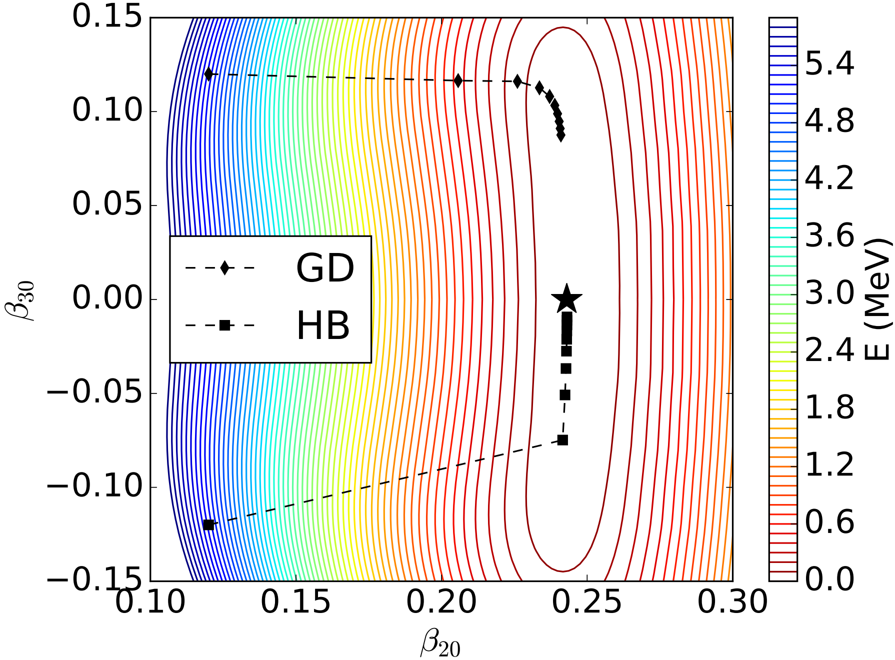


Possibilities





z
x
y


0.15
0.10
0.05
0.00
−0.05
−0.10
−0.15
0.10
0.15
0.20
0.25
0.30
β_{20}
β_{30}
GD
HB
5.4
4.8
4.2
3.6
3.0
2.4
1.8
1.2
0.6
0.0
E (MeV)