Rotational bands in the Thorium isotopes

Towards symmetry-unrestricted Skyrme-HFB with MOCCa

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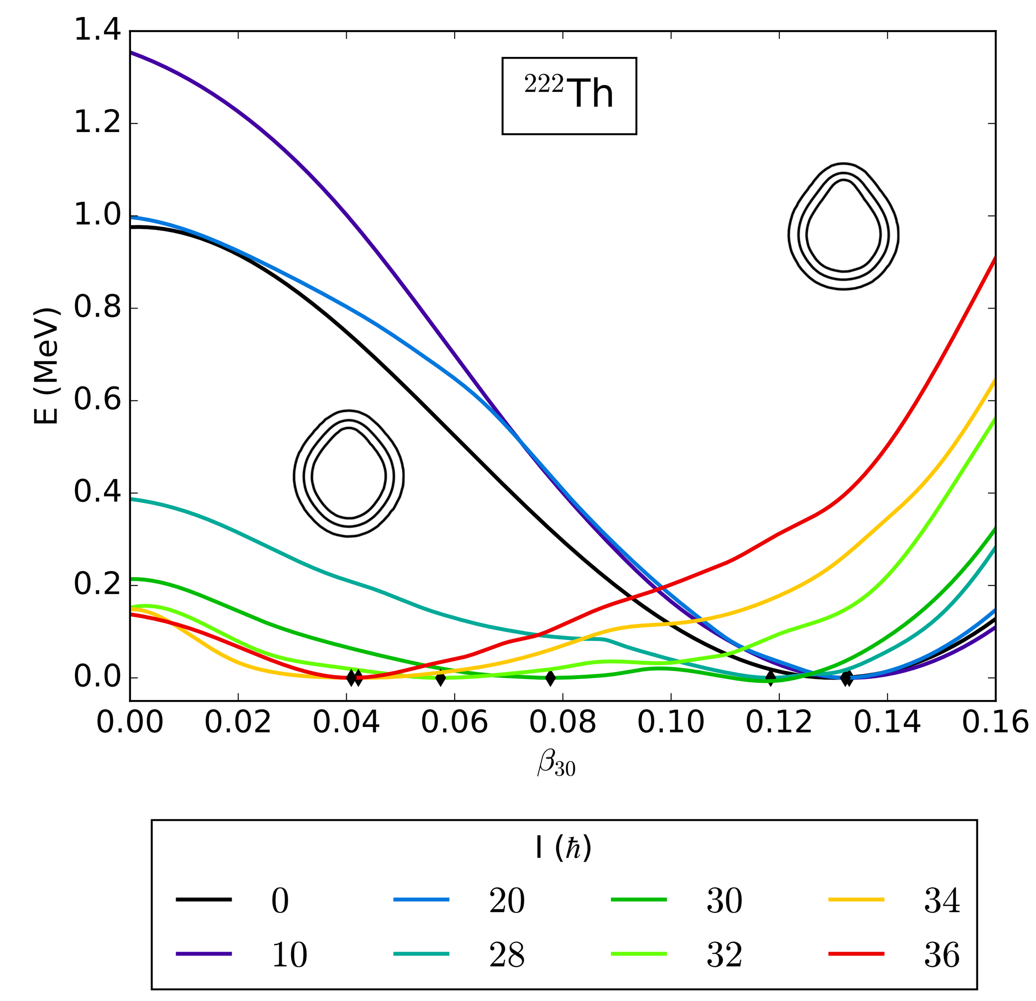
Ingredients

+ Skyrme functional: SLy5s1
  SLy5* with finetuned a_{surf} [1]
+ HFB(+LN) pairing
  Gradient method to find qp vacuum
  Fully self-consistent blocked qp for ^{223}Th (4)
+ Surface zero-range pairing interaction
+ Single-particle states in 3D coordinate space

= Numerical tool: **MOCCa** [2]
MOdular **C**ranking **C**ode
Large freedom of conserved and broken symmetries

Shape transition



Low spin, $0\hbar \leq I < 20\hbar$:
Pronounced octupole minimum at $\beta_{30} \approx 0.13$.
Studied with parity restoration for ^{224}Ra in [4].

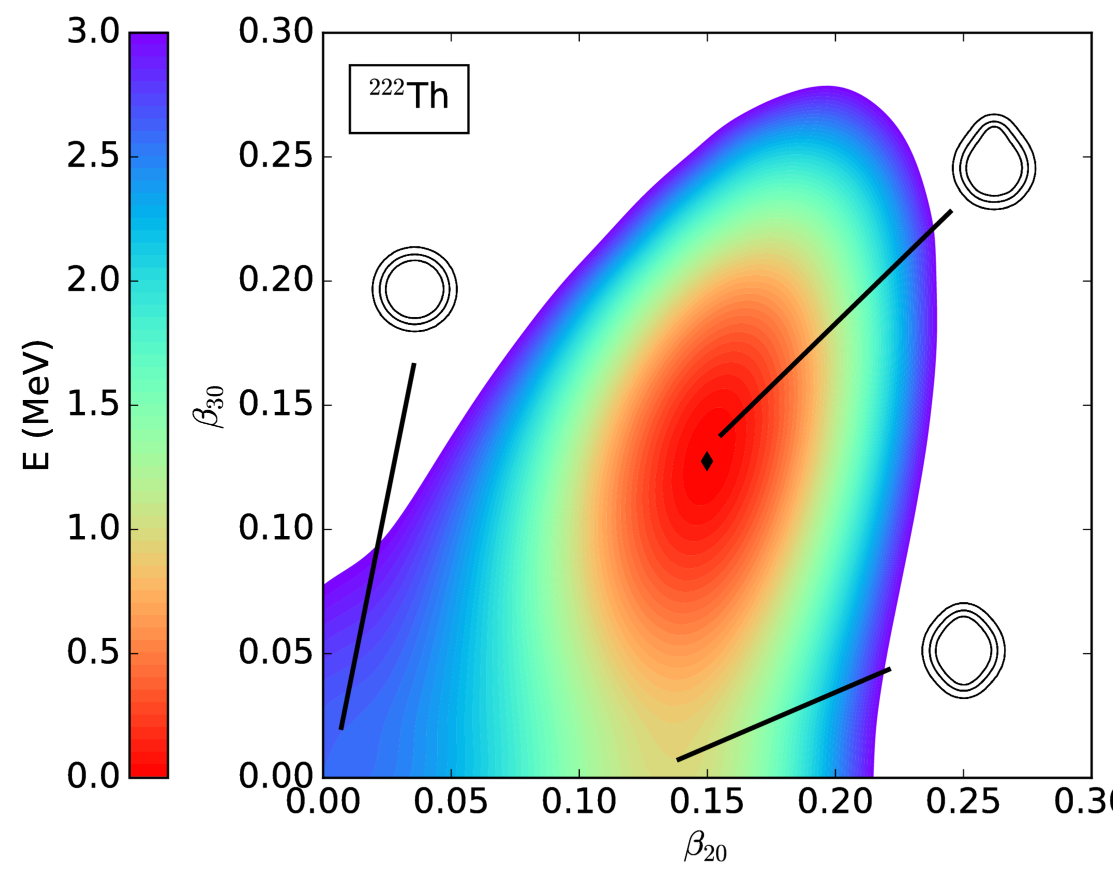
Medium spin, $20\hbar < I < 30\hbar$:
Quasi-symmetric shoulder/minimum appears.
Original minimum is much less pronounced.

High spin, $30\hbar < I$:
Quasi-symmetric minimum becomes global
The minimum at $\beta_{30} \approx 0.13$ vanishes
First described for ^{222}Th in [5].

Quadrupole & octupole

Th isotopes predicted with axially deformed minima.

	^{218}Th	^{220}Th	^{222}Th	^{224}Th	
Quadrupole β_{20}	0.00	0.11	0.15	0.17	(1)
Octupole β_{30}	0.00	0.10	0.13	0.15	(2)



Cranked Skyrme-HFB

Minimization of Routhian R instead of energy E [3]

$$E \rightarrow R = E - \omega_x \langle \hat{J}_x \rangle , \quad (3)$$

with ω_x a Lagrange multiplier used to satisfy

$$\langle \hat{J}_x \rangle = \sqrt{I(I+1)} .$$

The kinematic moment of inertia is

$$\mathcal{I}^{(1)} = \frac{I}{\omega_x} .$$

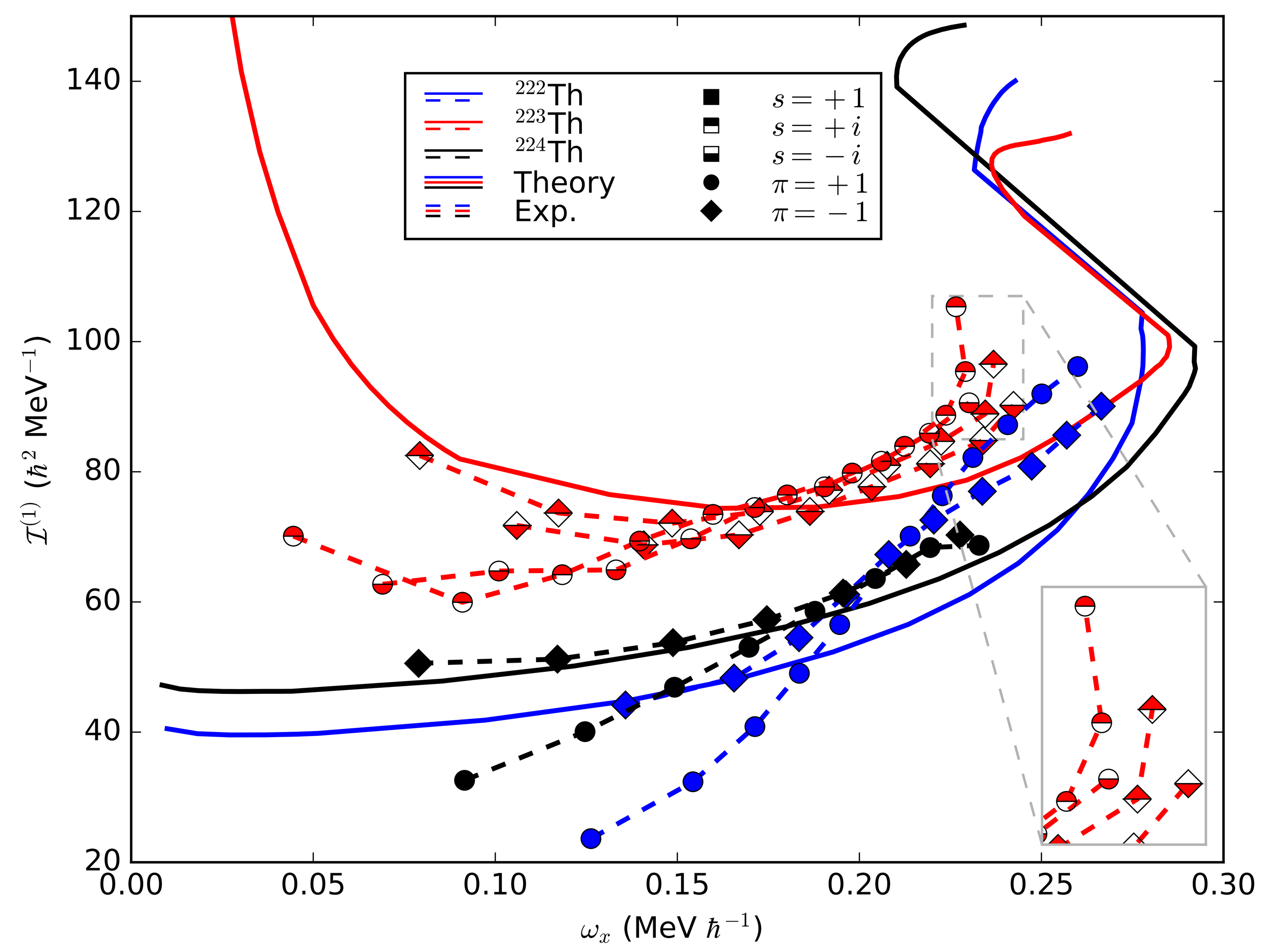
Broken symmetries

Symmetry	Q.N.	Freedom	See
Rotations	J	$\beta_{20} \neq 0$	(1)
Parity $\hat{P}$	π	$\beta_{30} \neq 0$	(2)
Axial rotations	K	$\langle \hat{J}_x \rangle \neq 0$	(3)
Signature $\hat{R}_x$	η_x	$\beta_{30} \neq 0$	(2)
Time-reversal	N.A.	$\langle \hat{J}_x \rangle \neq 0$	(3)
	N.A.	odd neutron	(4)

Simplex is the only label for single-particle states:

$$\hat{S}_x = \hat{P}\hat{R}_x$$

Moment of inertia: experiment suggests up/backbending



Up/backbend suggested at

	$\hbar\omega_{\text{theo}}$	$\hbar\omega_{\text{exp}}$	From
^{222}Th	0.29	> 0.25	[6, 7]
^{223}Th	0.28	~ 0.23	[8]
^{224}Th	0.27	N.A.	[9]

Experimentally, the observables are [10]

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

with different relations $I(J)$ for even-even or odd nuclei

$^{222/4}$Th: $I(J) = J$

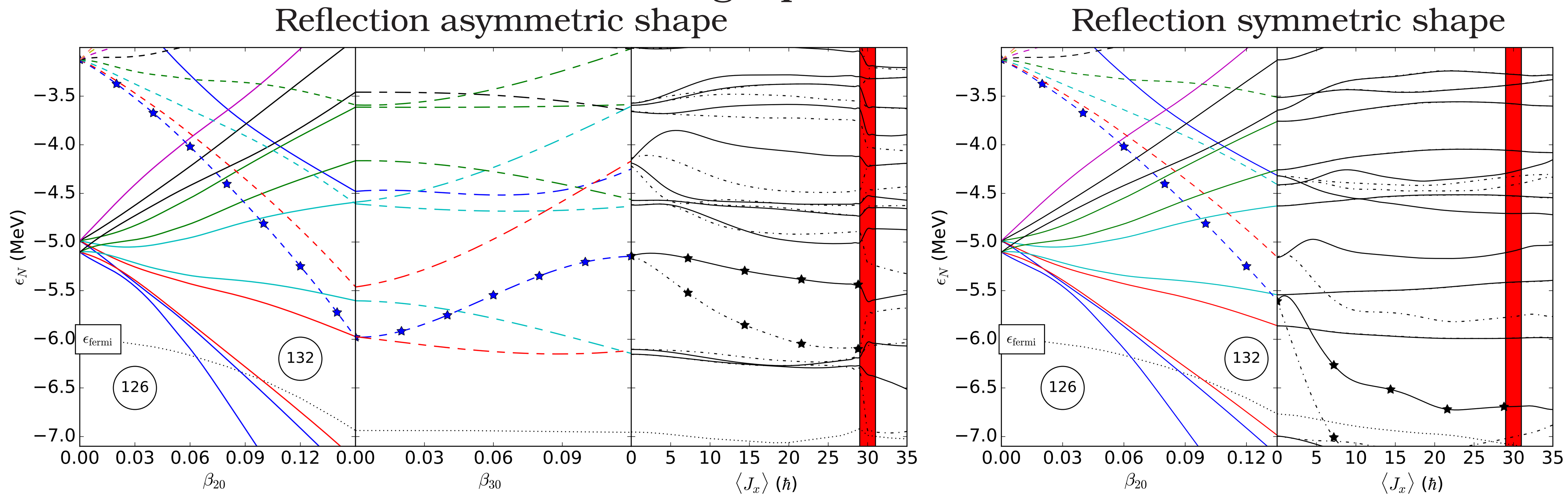
^{223}Th: $I(J) = \sqrt{\left(J + \frac{1}{2}\right)^2 - \left(\frac{5}{2}\right)^2} ,$

where the term $\left(\frac{5}{2}\right)^2$ represents the spin of the ground state.

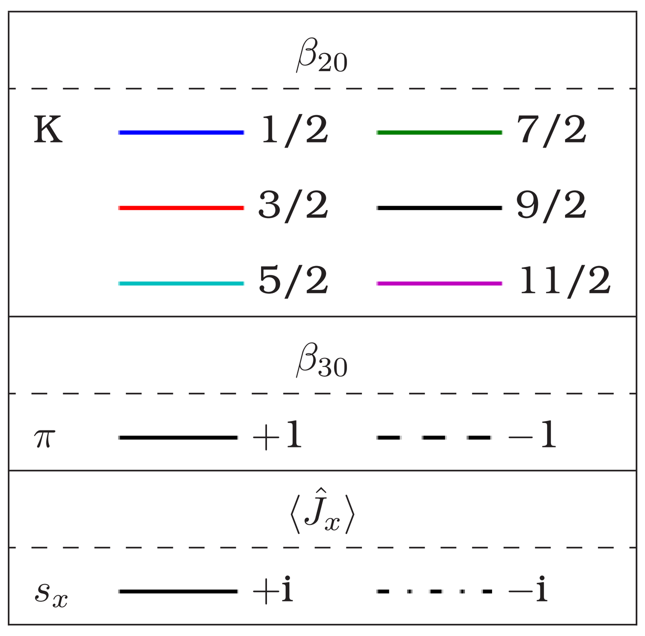
Single-particle properties of the competing shapes

Neutron single-particle routhians in ^{222}Th

Reflection asymmetric shape — Reflection symmetric shape



Intruder states $\nu(j15/2)$ ($\star$) and $\pi(i13/2)$ are crucial.



Reflection asymmetric:
Intruder states mix with natural parity orbitals.
When cranked, they repel due to parity mixing.
Thus, they stay away from the Fermi energy.

Reflection symmetric:
Intruder states do not mix with natural parity orbitals.
The low K intruders naturally have high $\langle \hat{J}_x \rangle$.
Cranking term rapidly aligns intruder $K \sim \frac{1}{2}$ orbitals.
Transition to a two-quasi-neutron, two-quasi-proton excitation.

Bonus: HFB without signature

A given set of Hartree-Fock-Bogoliubov quasi-particle operators defines an HFB vacuum

$$\left\{ \beta_j, \beta_j^\dagger \right\} \implies |\Psi^{\text{HFB}}_{\text{vac.}}\rangle .$$

With conserved antihermitian symmetry $\hat{R}_z$ we have

$$\hat{R}_z \hat{\beta}_j \hat{R}_z^\dagger = \eta \hat{\beta}_j , \quad \hat{R}_z \hat{\beta}_j^\dagger \hat{R}_z^\dagger = \eta^* \hat{\beta}_j^\dagger , \quad \eta = \pm i .$$

Problem:
Without conserved antihermitian symmetry, impossible to tell the difference when exchanging a quasi-particle for a quasi-hole.

$$\left. \begin{array}{l} \left\{ \beta_j, \beta_j^\dagger \right\} \implies |\Psi^1_{\text{vac.}}\rangle \\ \left\{ \beta_j^\dagger, \beta_j \right\} \implies |\Psi^2_{\text{vac.}}\rangle \end{array} \right\} ???$$

Solution:
Iteratively connect qp vacuum with symmetry-conserving vacuum via Thouless theorem

$$|\Psi^{(0)}_{\text{vac}}\rangle = |\Psi^{\text{sym}}_{\text{vac}}\rangle , \quad |\Psi^{(i+1)}_{\text{vac}}\rangle = \exp\left[-\frac{1}{2} \sum_{ij} Z_{ij} \hat{\beta}_i^\dagger \hat{\beta}_j^\dagger \right] |\Psi^{(i)}_{\text{vac}}\rangle .$$

Based on the same ideas as those used in Madrid [11, 12].

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