Nuclear shape dynamics at different energy scales

Nikolay Minkov

Institute of Nuclear Research and Nuclear Energy
Bulgarian Academy of Sciences, Sofia, Bulgaria
Research Group on Complex Deformed Atomic Nuclei

SDANCA-17, 6 October 2017

Contents

1. **Quadrupole-octupole core plus particle model**
   - Coherent quadrupole-octupole mode (CQOM)
   - Core plus particle coupling scheme. Coriolis interaction.
   - Model spectrum and transition probabilities
2. **The $3/2^+$ isomer phenomenon in the nucleus ^{229}Th**
3. **Quasi parity-doublet spectrum in ^{229}Th**
   - CQOM+DSM+BCS model calculation
   - Predicted B(E2) and B(M1) values for $3/2^+$ γ-decay
4. **Summary**

Quadrupole-octupole core plus particle Hamiltonian

$$H = H_{\mathrm{qo}} + H_{\mathrm{s.p.}} + H_{\mathrm{pair}} + H_{\mathrm{Coriol}}$$

$$H_{\mathrm{qo}} = -\frac{\hbar^2}{2B_2}\frac{\partial^2}{\partial\beta_2^2} - \frac{\hbar^2}{2B_3}\frac{\partial^2}{\partial\beta_3^2} + U(\beta_2,\beta_3,I)$$

$$U(\beta_2,\beta_3,I) = \frac{1}{2}C_2{\beta_2}^2 + \frac{1}{2}C_3{\beta_3}^2 + \frac{d_0 + \hat{I}^2 - \hat{I_z}^2}{2\mathcal{J}(\beta_2,\beta_3)}$$

$$H_{\mathrm{Coriol}} = -\frac{(\hat{I}_+\hat{j}_- + \hat{I}_-\hat{j}_+)}{2\mathcal{J}(\beta_2,\beta_3)}, \qquad \mathcal{J}(\beta_2,\beta_3) = (d_2\beta_2^2 + d_3\beta_3^2)$$

$$H_{\mathrm{sp}} = T + V_{\mathrm{ws}}(\beta_2,\beta_3,...) + V_{\mathrm{s.o.}} + V_{\mathrm{c}}$$

$$H_{qp} \equiv H_{\mathrm{s.p.}} + H_{\mathrm{pair}} \to \epsilon^K_{\mathrm{qp}} = \sqrt{(E^K_{\mathrm{sp}} - \lambda)^2 + \Delta^2}$$

Coherent quadrupole-octupole mode (CQOM) in the even core

$$U(\beta_2,\beta_3,I)+\langle H_{\mathrm{Coriol}}\rangle=\frac{1}{2}C_2{\beta_2}^2+\frac{1}{2}C_3{\beta_3}^2+\frac{\widetilde{X}(I,K)}{d_2\beta_2^2+d_3\beta_3^2}$$

$$\widetilde{X}(I,K)=[d_0+I(I+1)-K^2+2\mathcal{J}\langle H_K^c\rangle]/2$$

$$\beta_2=\sqrt{d/d_2}\eta\cos\phi\ ,\quad \beta_3=\sqrt{d/d_3}\eta\sin\phi\ ,\quad d=(d_2+d_3)/2$$

Coherent mode: $\omega=\sqrt{C_2/B_2}=\sqrt{C_3/B_3}\equiv\sqrt{C/B}$

$H_{\mathrm{qo}}+H_{\mathrm{Coriol}}\ \rightarrow$ **energy spectrum:**

$$E_{n,k}(I,K)=\hbar\omega\left[2n+1+\sqrt{k^2+b\widetilde{X}(I,K)}\right],\quad n=0,1,2,\ldots$$

Quadrupole-octupole vibration function of the core

$$\Phi^{\pi}_{n,k,I}(\eta,\phi)=\psi^{I}_{nk}(\eta)\varphi^{\pi}_{k}(\phi)$$

$$\psi^{I}_{nk}(\eta)=\sqrt{\frac{2c\Gamma(n+1)}{\Gamma(n+2s+1)}}e^{-c\eta^2/2}c^{s}\eta^{2s}L^{2s}_{n}(c\eta^2)$$

$$\begin{aligned}\varphi^{+}_{k}(\phi) &= \sqrt{2/\pi}\cos(k\phi)\ , \quad k=1,3,5,\ldots\\ \varphi^{-}_{k}(\phi) &= \sqrt{2/\pi}\mathbf{sin}(k\phi)\ , \quad k=2,4,6,\ldots\end{aligned}$$

[N. M. et al, Phys. Rev. C **73**, 044315 (2006); **76**, 034324 (2007)]

Total core plus particle wave function

$$\begin{aligned}\Psi^{\pi,\pi^b}_{nkIMK}(\eta,\phi) &= \frac{1}{2}\sqrt{\frac{2I+1}{16\pi^2}}\Phi^{\pi\cdot\pi^b}_{nkI}(\eta,\phi)\\ &\times \left[D^I_{M\,K}(\theta)\mathcal{F}^{(\pi^b)}_K + \pi\cdot\pi^b(-1)^{I+K}D^I_{M\,-K}(\theta)\mathcal{F}^{(\pi^b)}_{-K}\right]\end{aligned}$$

$\pi^b = \pm$ experimental parity of the bandhead state

$\pi_c = \pi\cdot\pi^b = (+) \rightarrow \Phi^{+}_{\text{core}} \Rightarrow$ downwards shifted levels

$\pi_c = (-) \rightarrow \Phi^{-}_{\text{core}} \Rightarrow$ upwards shifted energy sequence

$\mathcal{F}^{(\pi^b)}_K = \mathcal{F}^{(\pm)}_K \rightarrow$ projected s.p. wave function

[N. M., S. Drenska, M. Strecker and W. Scheid, JPG **37**, 025103 (2010)]

Quasi parity-doublet spectrum from CQOM+DSM+BCS

$$E_{nk}(I^{\pi},K_b) = \epsilon_{\mathrm{qp}}^{K_b} + \hbar\omega\left[2n+1+\sqrt{k^2+b\widetilde{X}(I^{\pi},K_b)}\right]$$

$$\begin{aligned}\widetilde{X}(I^{\pi},K_b) &= \frac{1}{2}\Bigg[d_0 + I(I+1) - K_b^2 + (-1)^{I+\frac{1}{2}}\left(I+\frac{1}{2}\right)a_{\frac{1}{2}}^{(\pi\pi^b)}\delta_{K_b,\frac{1}{2}} \\ &\quad - A\sum_{\substack{\nu\neq b \\ (K_\nu=K_b\pm 1,\frac{1}{2})}}\frac{\left[\widetilde{a}_{K_\nu K_b}^{(\pi\pi^b)}(I)\right]^2}{\epsilon^{K_\nu}-\epsilon^{K_b}}\Bigg]\end{aligned}$$

$A \equiv 1/[2\mathcal{J}(\beta_2^0,\beta_3^0)] \rightarrow$ K- mixing constant

$\widetilde{a}_{K_\nu K_b}^{(\pi,\pi^b)}(I) \rightarrow$ Coriolis mixing factors

$a_{1/2}^{(\pi,\pi^b)} = \pi\pi_b a_{\frac{1}{2}-\frac{1}{2}}^{(\pi^b)} \rightarrow$ decoupling factor

[N. M., Phys. Scripta **T154**, 014017 (2013)]

Coriolis mixed core+particle wave function

$$\widetilde{\Psi}^{\pi,\pi^b}_{nkIMK_b} = \frac{1}{\widetilde{N}_{I\pi K_b}} \left[\Psi^{\pi,\pi^b}_{nkIMK_b} + A \sum_{\substack{\nu\neq b \\ (K_\nu = K_b \pm 1, \frac{1}{2})}} C^{I\pi}_{K_\nu K_b} \Psi^{\pi,\pi^b}_{nkIMK_\nu} \right]$$

$$C^{I\pi}_{K_\nu K_b} = \frac{\widetilde{a}^{(\pi\pi^b)}_{K_\nu K_b}(I)}{\epsilon^{K_\nu} - \epsilon^{K_b}}$$

Reduced $E\lambda$ transition probabilities

$$B(E\lambda;\pi^{b_i} n_i k_i I_i K_i \to \pi^{b_f} n_f k_f I_f K_f) = \frac{1}{2I_i+1}\sum_{M_i M_f \mu}\left|\left\langle \widetilde{\Psi}^{\pi_f,\pi^{b_f}}_{n_f k_f I_f M_f K_f}\right|\hat{\mathcal{M}}_\mu(E\lambda)\left|\widetilde{\Psi}^{\pi_i,\pi^{b_i}}_{n_i k_i I_i M_i K_i}\right\rangle\right|^2$$

$$\hat{\mathcal{M}}_\mu(E\lambda) = \sqrt{\frac{2\lambda+1}{4\pi(4-3\delta_{\lambda,1})}}\,Q_{\lambda 0}\Sigma_\nu D^\lambda_{\mu\nu}$$

$$\lambda = 1,2,3, \quad \mu = 0,\pm 1,\ldots,\pm\lambda$$

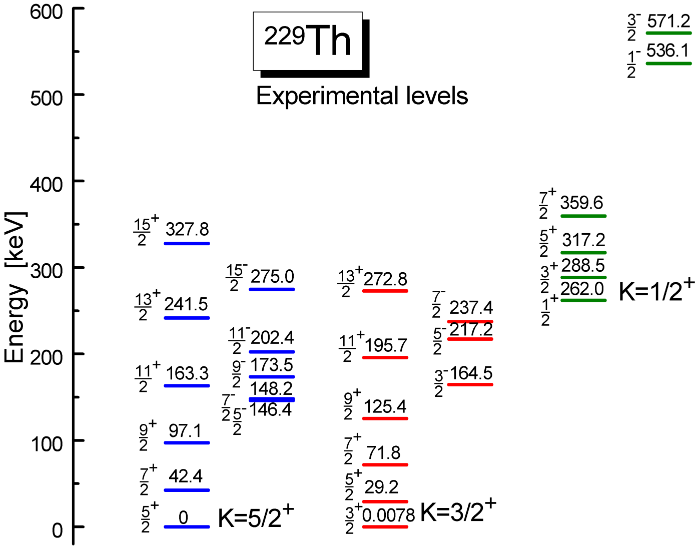
$$\hat{Q}_{\lambda 0} \equiv \hat{Q}_{\lambda 0}(\beta_2,\beta_3) \equiv \hat{Q}_{\lambda 0}(\eta,\phi)$$

Reduced $M1$ transition probabilities

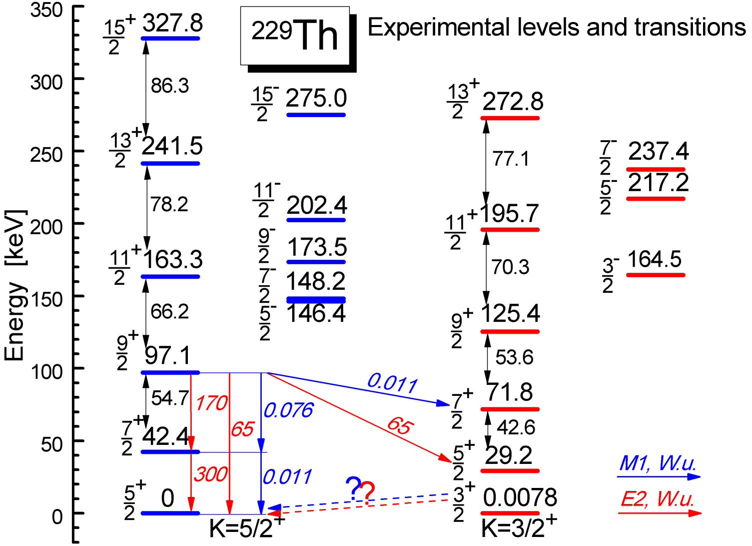
$$\hat{M}1 = \sqrt{\frac{3}{4\pi}}\mu_N[g_R(\hat{I} - \hat{j}) + g_s\,\hat{s} + g_l\,\hat{l}]$$

$$\begin{aligned}\langle \mathcal{F}_{K_f}^{(\pi^{b_f})}|\hat{M}1_z|\mathcal{F}_{K_i}^{(\pi^{b_i})}\rangle &= \sqrt{\frac{3}{4\pi}}\mu_N\left[(g_l - g_R)K_i\delta_{K_fK_i}\langle \mathcal{F}_{K_f}^{(\pi^{b_f})}|\mathcal{F}_{K_i}^{(\pi^{b_i})}\rangle\right.\\ &+ \left.(g_s - g_l)\langle \mathcal{F}_{K_f}^{(\pi^{b_f})}|\hat{s}_z|\mathcal{F}_{K_i}^{(\pi^{b_i})}\rangle\right]\end{aligned}$$

^{229}Th: experimental spectrum



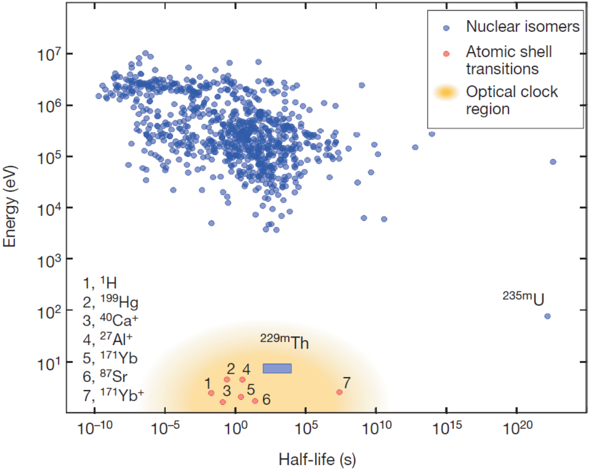
^{229}Th: Low-energy levels and transitions



^{229}Th: $3/2^+$ isomer possible applications

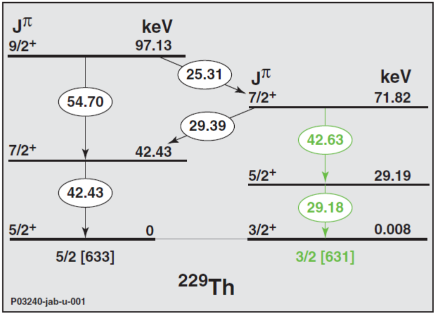
✓ Phenomena on the border between nuclear and atomic physics
✓ Nuclear quantum optics with X-ray laser pulses [T. Bürvenich et al., PRL **96**, 142501 (2006)]
✓ Nuclear γ-ray laser of optical range [E. Tkalya, PRL **106**, 162501 (2011)]
✓ Nuclear clock with a total fractional inaccuracy approaching $1 \times 10^{-19} - 10^{-20}$ outperforming the existing atomic-clock technology [C. J. Campbell et al., PRL **108**, 120802 (2012)]
✓ $\Rightarrow$ Investigation of possible time variations of fundamental constants (fine structure constant $\alpha = e^2/\hbar c$; strong interaction parameter $m_q/\Lambda_{\mathrm{QCD}}$): Unification theories $\rightarrow$ cosmology $\rightarrow$ variation of the fundamental constants in the expanding Universe (quasar absorption spectra, big bang nucleosynthesis) [V. V. Flambaum, PRL **97**, 092502 (2006)]

Energy-half-life distribution

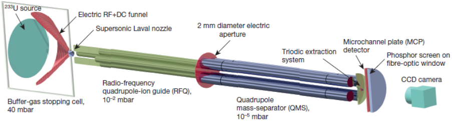


L. von der Wense *et al.*, Nature **533**, 47 (2016)

^{229}Th, $3/2^+$ isomer: energy estimates and decay detection



L. Kroger, C. Reich, NPA **259**, 29 (1976), $E(^{229m}Th) < 100$eV
D.Burke et al, PRC1990,NPA2008
R. Helmer, C. Reich, PRC **49**, 1845 (1994), $E(^{229m}Th) \sim 3.5$eV
Last energy estimate:
$E(^{229m}Th) =$
$(29.39 - 29.18) - (42.63 - 42.43)$
~ 0.0078 keV
B. Beck et al, PRL **98**, 142501 (2007); LLNL-PROC-415170 (2009)



Decay detection:
L. von Wense et al, Nature **533**, 47 (2016), $\tau\ (^{229m}\mathrm{Th}^{2+}) \gtrsim 60$s
B. Seiferle et al, PRL **118**, 042501 (2017), $\tau\ (^{229m}\mathrm{Th})\ 7 \pm 1\mu s$

^{229}Th, $3/2^+$ isomer: estimates of transition probabilities

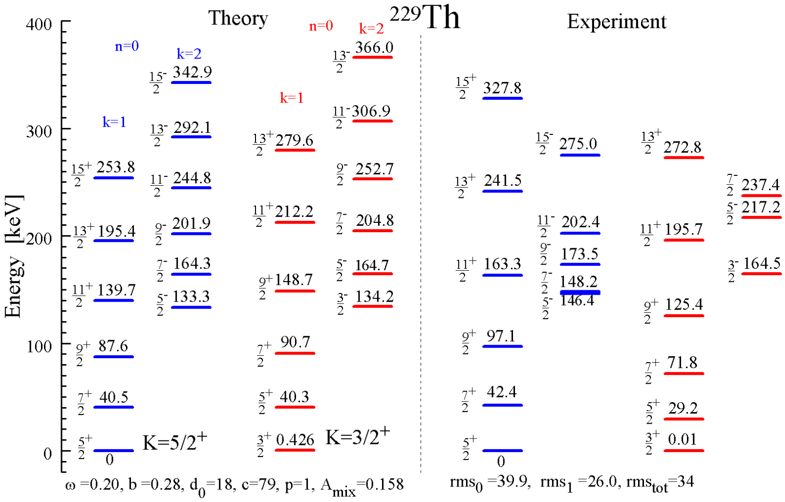
• Phenomenological calculations using available data for M1 and E2 transitions → branching ratios, Alaga rules [A. Dykhne, E. Tkalya, JETP Lett. **67**, 251 (1998); E. Tkalya, PRC **92**, 054324 (2015)] ⇒ B(M1)= 0.048 W.u. currently quoted value
✓ *E*2 decay channel disregarded in the internal conversion process
✓ Role of the Coriolis mixing diminished

• QPM calculations [K. Gulda *et al.*, NPA **703**, 45 (2002); E. Ruchowska *et al.*, PRC **73**, 044326 (2006)]
$B(M1; 3/2^+ \rightarrow 5/2^+) = 0.014$ W.u.
$B(E2; 3/2^+ \rightarrow 5/2^+) = 67$ W.u.
No particular analysis/interpretation of the $3/2^+$ isomeric state proposed

Details of the CQOM+DSM+BCS model calculations

- General: 2 quasi-doublets with identical collective quantum numbers $n = 0$, $k^+ = 1$, $k^- = 2$ built on 5/2[633] and 3/2[631] Nilsson s.p. orbital
- DSM: β_2 and β_3 determination $\rightarrow$ correct positions and mutual spacing of the 5/2[633] and 3/2[631] orbitals $\Rightarrow$ $\beta_2 = 0.240$ and $\beta_3 = 0.115$
- CQOM: parameters fits $\rightarrow$ ω, b, d_0 (for energy levels); c, p (transition probabilities); K-mixing constant A (energies and transitions)
- BCS: pairing constants tuning $\rightarrow$ $g_0 = 18.805$, $g_1 = 7.389$ $\Rightarrow$ $E(3/2^+) \sim 0.4$ keV
- Possible further refinement: ω - oscillator tuning $\Rightarrow$ $E(3/2^+) \sim 0.0078$ keV $\rightarrow$ rms deterioration $0.4 - 1.0$ keV

Theoretical and experimental quasi parity-doublet spectrum of ^{229}Th



Theoretical and experimental B(E2) and B(M1) transition values for ^{229}Th

N. M. and A. Pálffy, Phys. Rev. Lett. **118**, 212501 (2017)

Type/Mult	Transition	Th1[Th2] (W.u.)	Exp (W.u.)
E2	$7/2^+_{yrs} \rightarrow 5/2^+_{yrs}$	252 [267]	300 ($\pm$16)
E2	$9/2^+_{yrs} \rightarrow 5/2^+_{yrs}$	82 [85]	65 ($\pm$7)
E2	$9/2^+_{yrs} \rightarrow 7/2^+_{yrs}$	213 [224]	170 ($\pm$30)
E2	$9/2^+_{yrs} \rightarrow 5/2^+_{ex1}$	19.98 [17.37]	6.2 ($\pm$0.8)
E2	$\mathbf{3/2^+_{ex1} \rightarrow 5/2^+_{yrs}}$	27.04 [23.05]	?
M1	$7/2^+_{yrs} \rightarrow 5/2^+_{yrs}$	0.0093 [0.0085]	0.0110 ($\pm$0.0040)
M1	$9/2^+_{yrs} \rightarrow 7/2^+_{yrs}$	0.0178 [0.0157]	0.0076 ($\pm$0.0012)
M1	$9/2^+_{yrs} \rightarrow 7/2^+_{ex1}$	0.0151 [0.0130]	0.0117 ($\pm$0.0014)
M1	$\mathbf{3/2^+_{ex1} \rightarrow 5/2^+_{yrs}}$	0.0076 [0.0061]	?

Th1 $\rightarrow E(3/2^+) = 0.4263$ keV

Th2 $\rightarrow E(3/2^+) = 0.0078$ keV

Theoretical B(E2) and B(M1) transition values for ^{229}Th at different parameter sets

ω	b	d_0	c	p	A	$k_{\mathrm{yr}}^{(-)}$	$k_{\mathrm{ex}}^{(-)}$	rms$_{\mathrm{yr}}$	rms$_{\mathrm{ex}}$	rms$_{\mathrm{tot}}$	$E_{\mathrm{ex}}(\frac{3}{2}^+)$	$B(E2)$	$B(M1)$
0.2039	0.28	18	79	1.0	0.158	2	2	39.9	26.0	34	0.4263	27.04	0.0076
0.2361	0.28	33	89	1.0	0.141	2	2	41.2	26.4	35	0.0078	23.05	0.0061
0.0912	2.39	49	245	1.0	0.152	4	6	37.6	15.8	29	0.3556	25.80	0.0071
0.0635	4.51	45	321	1.0	0.144	6	8	36.4	12.4	28	0.0725	22.86	0.0063
0.0563	7.34	66	473	1.0	0.138	8	10	38.3	11.9	29	10^{-9}	21.31	0.0058

$\Rightarrow$ experimental transition probabilities for the $3/2^+$-isomer decay in ^{229}Th expected in the limits:

$B(E2)$=20–30 W.u.
$B(M1)$=0.006–0.008 W.u.

Phys. Rev. Lett. **118**, 212501 (2017)

First application to IC rates and lifetimes estimation

$$\Gamma_{\mathrm{IC}}^{\mathrm{M1}} = \frac{8\pi^2}{9} B_{\downarrow}(\mathrm{M1}) \sum_{\kappa} (2j+1)(\kappa_i + \kappa)^2 \begin{pmatrix} j_i & j & 1 \\ 1/2 & -1/2 & 0 \end{pmatrix}^2 |R_{\varepsilon\kappa}^{\mathrm{M1}}|^2$$

$$\Gamma_{\mathrm{IC}}^{\mathrm{E2}} = \frac{8\pi^2}{25} B_{\downarrow}(\mathrm{E2}) \sum_{\kappa} (2j+1) \begin{pmatrix} j_i & j & 1 \\ 1/2 & -1/2 & 0 \end{pmatrix}^2 |R_{\varepsilon\kappa}^{\mathrm{E2}}|^2$$

- Reduced probability $B_{\downarrow} = \frac{|\langle I_g \| \hat{\mathcal{M}} \| I_e \rangle|^2}{2I_e+1}$ denotes the averaged probability of nuclear transition from isomeric to ground state
- Radial integral $R_{\varepsilon\kappa}$

$$R_{\varepsilon\kappa}^{\mathrm{M1}} = \int_0^{\infty} dr \Big(g_{n_i\kappa_i}(r) f_{\varepsilon\kappa}(r) + g_{\varepsilon\kappa}(r) f_{n_i\kappa_i}(r) \Big)$$

$$R_{\varepsilon\kappa}^{\mathrm{E2}} = \int_0^{\infty} \frac{dr}{r} \Big(g_{n_i\kappa_i}(r) g_{\varepsilon\kappa}(r) + f_{\varepsilon\kappa}(r) f_{n_i\kappa_i}(r) \Big)$$

Lifetimes of excited electronic states in ^{229}Th$^+$ calculated through the isomer B(M1) and B(E2) values

Ion charge	Configuration	Energy (cm^{-1})	Lifetime
1+	$5f6d^2$	30 223	0.4 s
	$7s^27p$	31 626	40 ns
2+	$5f7s$	7501	20 μs
	$6d7s$	16 038	100 ns

P. Bilous, G. Kazakov, I. Moore, T. Schumm and A. Pálffy, PRA **95**, 032503 (2017)

$B(E2)$=29 W.u. from the CQOM calculations

SUMMARY

- Model: collective CQOM plus microscopic DSM+BCS with fully taken into account Coriolis interaction - fully derived model expressions for energy and E/M transition probabilities
- Application: complete nuclear-structure-model calculation for the low-lying ^{229}Th spectrum including the $3/2^+$ isomer (octupole-shape driven parity quasi-doublet structure)
- $3/2^+$ state interpretation: a bandhead of an excited parity quasi-doublet, built on 3/2[631] q.p. state coupled to a collective quadrupole-octupole vibration mode and rotation motion - remarkably fine interplay between all these modes!
- Result: description of the available data on energy and transition probabilities; model predicted B(E2) and B(M1) values for $3/2^+_{ex1} \rightarrow 5/2^+_{yrs}$ transitions
- Questions: 1) To what extent nuclear shape dynamics can drive effects in the atomic energy scale? 2) Could we expect the same in other nuclei?