Theoretical predictions for the decay rates and magnetic moment in ^{229m}Th

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HINPW5, 13 April 2019

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Support:

Deutsche Forschungsgemeinschaft

BgNSF (Contracts No. DFNI-E02/6 and KP-06-N28/6)

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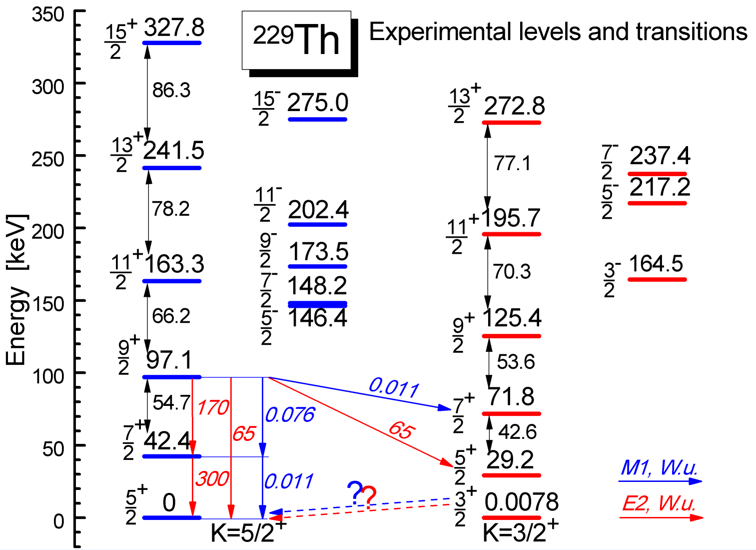


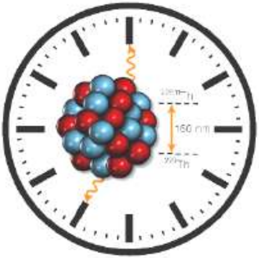
^{229}Th: Nuclear clock

The thorium isomer

Use a nuclear transition for a "nuclear clock"?

$^{229m}\mathrm{Th} \quad \Delta E/E \simeq 10^{-20}$

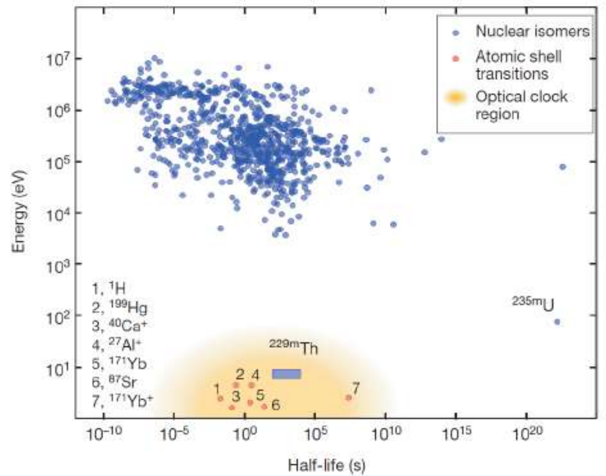
7.8 eV, λ ~ 160 nm
M1 (+E2) transition



ISOLATION FROM ENVIRONMENT

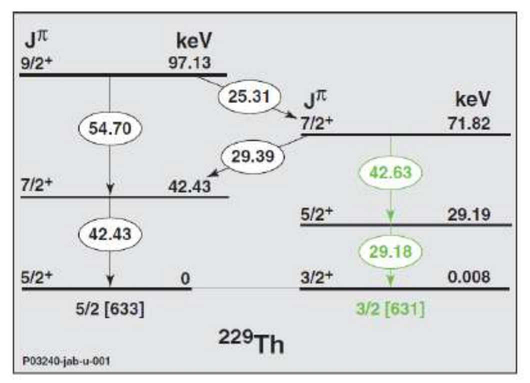
- Better frequency standard
- Variation of fundamental constants
- Oscillator involving the strong force

Energy-half-life distribution



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

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



L. Kroger, C. Reich, NPA1976, $E(^{229m}Th) < 100$eV

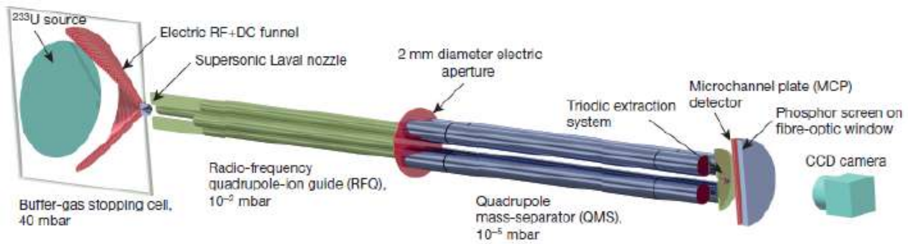
D. Burke et al, PRC1990, NPA2008

R. Helmer, C. Reich, PRC1994, $E(^{229m}Th) \sim 3.5$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)

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



Decay detection:

L. von Wense, ..., P. Thirolf et al, Nature **533**, 47 (2016), τ (^{229m}Th^{2+}) $\gtrsim$ 60s

B. Seiferle, ..., P. Thirolf et al, PRL **118**, 042501 (2017), τ (^{229m}Th) $7 \pm 1\mu$s

J. Thielking, ..., P. Thirolf et al, Nature **556**, 321 (2018), μ (^{229m}Th) $-0.37(6)\mu_N$

^{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)]
✓ ⇒ Investigation of possible time variations of fundamental constants (fine structure constant $\alpha = e^2/\hbar c$; strong interaction parameter m_q/Λ_{QCD}): Unification theories → cosmology → variation of the fundamental constants in the expanding Universe (quasar absorption spectra, big bang nucleosynthesis) [V. V. Flambaum, PRL **97**, 092502 (2006)]

Quadrupole-octupole core plus particle Hamiltonian

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

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

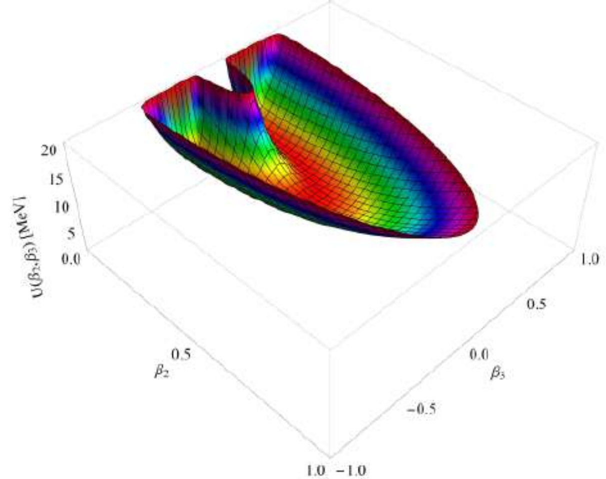
$$U(\beta_2,\beta_3,I) = \frac{1}{2}C_2{\beta_2}^2 + \frac{1}{2}C_3{\beta_3}^2 + \frac{d_0 + \hat{I}^2 - {\hat{I}_z}^2}{2\mathcal{J}(\beta_2,\beta_3)}$$

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

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

$$H_{qp} \equiv H_{\text{s.p.}} + H_{\text{pair}} \rightarrow \epsilon_{\text{qp}}^K = \sqrt{(E_{\text{sp}}^K - \lambda)^2 + \Delta^2}$$

Quad.-oct. potential of a coherent mode $\omega = \sqrt{C_2/B_2} = \sqrt{C_3/B_3}$



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

Total core plus particle wave function

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

$\Phi^{\pi}_{n,k,I}(\eta,\phi) = \psi^I_{nk}(\eta)\varphi^{\pi}_k(\phi) \rightarrow$ quad.-oct. vib. function of the core

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

$\mathcal{F}_K^{(\pi^b)} = \mathcal{F}_K^{(\pm)} \rightarrow$ π- projected s.p. w. function (π^b exp. bh parity)

$$N_K^{(\pi^b)} = \left[\left\langle \mathcal{F}_K^{(\pi^b)} \middle| \mathcal{F}_K^{(\pi^b)} \right\rangle\right]^{\frac{1}{2}}$$

Quasi parity-doublet spectrum from CQOM+DSM+BCS+Coriol

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

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

$$\widetilde{\Psi}_{nkIMK_b}^{\pi,\pi^b} = \frac{1}{\widetilde{N}_{I\pi K_b}}\left[\Psi_{nkIMK_b}^{\pi,\pi^b} + A\sum_{\nu\neq b} C_{K_\nu K_b}^{I\pi}\Psi_{nkIMK_\nu}^{\pi,\pi^b}\right]$$

$$C_{K_\nu K_b}^{I\pi} = \frac{\widetilde{a}_{K_\nu K_b}^{(\pi\pi^b)}(I)}{\epsilon^{K_\nu} - \epsilon^{K_b}} \qquad \widetilde{a}_{K_\nu K_b}^{(\pi,\pi^b)}(I) \sim \langle\mathcal{F}_{K_\nu}^{(\pi^b)}|\hat{j}_+|\mathcal{F}_{K_b}^{(\pi^b)}\rangle \;\rightarrow K\text{-mixing}$$

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

Reduced $E\lambda$ (λ=1,2,3) and $M1$ transition probabilities

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

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

Coriolis K-mixed matrix elements $\Rightarrow$ permission of gamma transitions with $K_f \neq K_i$ (forbidden by the axial symmetry)

Magnetic moment in a s.p./q.p. state with $K = K_{bh}$

$$\hat{M}1 = \sqrt{\frac{3}{4\pi}}\mu_N[g_R(\hat{I} - \hat{j}) + g_s\,\hat{s} + g_l\,\hat{l}], \quad \hat{j} = \hat{l} + \hat{s}, \quad \mu_N = \frac{e\hbar}{2mc}$$

$$\mu = \sqrt{\frac{4\pi}{3}}\langle\widetilde{\Psi}_{IIK_b}|\hat{M}1_z|\widetilde{\Psi}_{IIK_b}\rangle$$

$g_s = q_s \cdot g_s^{free}$

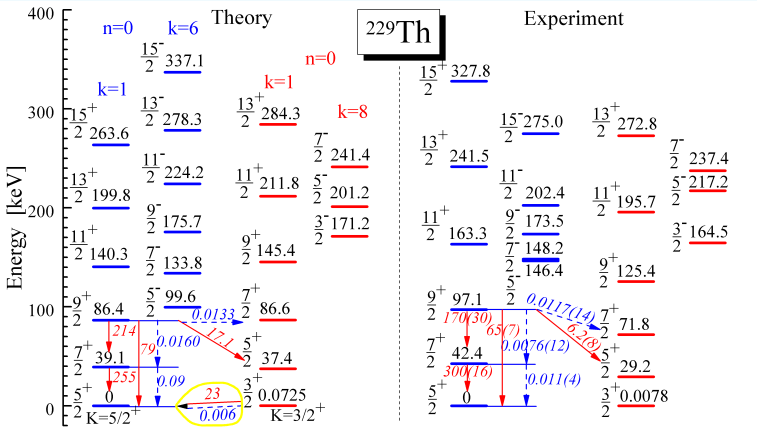
spin gyromagnetic quenching (core polarization effect): $q_s = 0.6$

$g_R = q_R \cdot Z/A$

collective gyromagnetic quenching (pairing effect):

q_R=1.0, **0.8** (from exp. M1/E2), **0.7** (Nilsson), **0.6** (HF+BCS)

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



DSM: s.p. orbitals GS(5/2[633]), IS(3/2[631]); $\beta_2 = 0.240$, $\beta_3 = 0.115$

BCS: $g_0 = 18.8$, $g_1 = 7.4$

CQOM: $\omega = 0.06$ MeV$/\hbar$, $b = 4.5\ \hbar^{-2}$, $d_0 = 45\ \hbar^2$, $c = 320$, $p = 1$

Coriol: $A = 0.144$ keV

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

ω	b	d_0	c	p	A	$k_{yr}^{(-)}$	$k_{ex}^{(-)}$	rms$_{yr}$	rms$_{ex}$	rms$_{tot}$	$E_{ex}(\frac{3}{2}^+)$	$B(E2)$	$B(M1)$
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

$\Rightarrow$ 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.

N. M. and A. Pálffy, Phys. Rev. Lett. **118**, 212501 (2017)
N. M. Bulg. J. Phys. **44**, 434 (2017)
P. Bilous, N.M. and A. Pálffy, PRC **97**, 044320 (2018) [predictions for M1 and E2 internal conversion rates]

Magnetic moments (in μ_N) in the $3/2^+_{\mathrm{IS}}$ and $5/2^+_{\mathrm{GS}}$ states of ^{229}Th

N. Minkov and A. Pálffy, Phys. Rev. Lett., in press (2019)

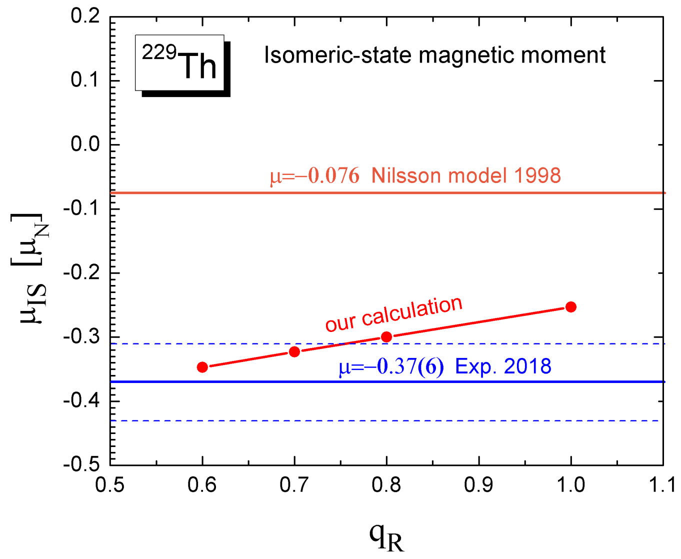
μ	q_R (our work)				other theories		laser spectroscopy			
	1.0	0.8	0.7	0.6	Th77	Th98	Exp74	Exp13	Exp18a	Exp18b
μ_{GS}	0.654	0.591	0.559	0.528	0.54	–	0.46(4)	0.360(7)	–	–
μ_{IS}	−0.253	−0.300	−0.323	−0.347	–	−0.076	–	–	(−0.3)-(−0.4)	−0.37(6)

Th77: Modified Woods-Saxon Model,
R. Chasman et al, Rev. Mod. Phys. **49**, 833 (1977)

Th98: Nilsson Model,
A. Dykhne and E. Tkalya, JETP Lett. **67**, 251 (1998)

Exp74: S. Gerstenkorn et al., J. Phys. (Paris) **35**, 483 (1974)
Exp13: M. Safronova et al, Phys. Rev. A **88**, 060501(R) (2013)
Exp18a: R. Müller et al., Phys. Rev. A **98**, 020503(R) (2018)
Exp18b: J. Thielking,..., P.Thirolf, E.Peik, Nature **556**, 321 (2018)

Magnetic moment (in μ_N) in the $3/2^+_{\mathrm{IS}}$ state of ^{229}Th

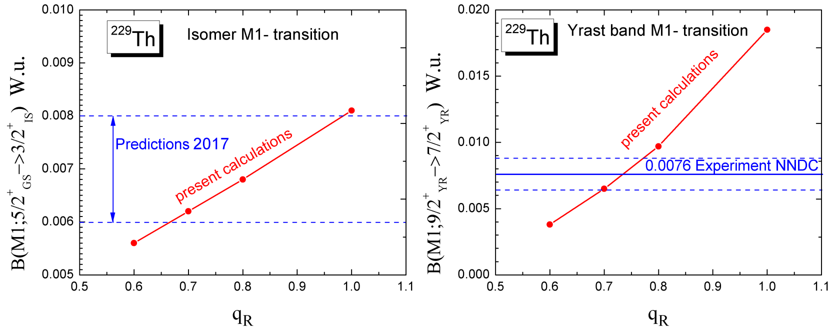


Predicted $B(M1)$ values (in W.u.) for ^{229}Th in dependence of q_R

Decay	q_R				Experiment
	1.0	0.8	0.7	0.6	
$\frac{3}{2}^+_{ex} \rightarrow \frac{5}{2}^+_{yr}$	0.0081	0.0068	0.0062	0.0056	–
$\frac{7}{2}^+_{yr} \rightarrow \frac{5}{2}^+_{yr}$	0.0096	0.0043	0.0025	0.0011	0.0110 (40)
$\frac{9}{2}^+_{yr} \rightarrow \frac{7}{2}^+_{yr}$	0.0185	0.0097	0.0065	0.0038	0.0076 (12)
$\frac{9}{2}^+_{yr} \rightarrow \frac{7}{2}^+_{ex}$	0.0144	0.0147	0.0149	0.0151	0.0117 (14)

N. Minkov and A. Pálffy, Phys. Rev. Lett., in press (2019)

Predicted $B(M1)$ values (in W.u.) for ^{229}Th in dependence of q_R



$\Rightarrow \mu_{GS}, \mu_{IS}$ constraints in the determination of isomer decay rates

Concluding remarks

- Model: CQOM+DSM+BCS with Coriolis mixing – description of K-suppressed EM transitions at axial symmetry
- ^{229}Th spectrum: $\rightarrow$ quadrupole-octupole-shape driven quasi parity-doublet structure built on 5/2[633], 3/2[631] qp states
- 7.8 eV $3/2^+$ isomer interpretation: a bandhead of an excited quasi parity-doublet, built on 3/2[631] q.p. state coupled to a collective quadrupole-octupole vibration mode and rotation motion – very fine interplay between all these modes
- Predictions for: B(E2) and B(M1) isomer decay probabilities; Magnetic dipole moment $\Rightarrow$ surprisingly good reproduction of $\mu_{\mathrm{IS}}^{\mathrm{exp}}$, further constraint on model conditions [$\mu_{\mathrm{GS}}^{\mathrm{exp}}$]
- Questions: To what extent nuclear shape dynamics can govern the EM properties of ^{229}Th and its 7.8 eV isomer? Could we expect similar properties in other nuclei, e.g. ^{235m}U?