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Electromagnetic Properties of the ^{229m}Th Isomer

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Abstract. We study the magnetic and electric radiative decay properties of the 7.8 eV ^{229m}Th isomer within a model of nuclear collective quadrupole-octupole and single particle (s.p.) motions with Coriolis interaction. We examine a number of possible values for the magnetic dipole moment (MDM) in the $K = 5/2^+$ ground and the $K = 3/2^+$ isomeric states based on the parity-projected s.p. wave functions obtained for the unpaired neutron in both states by using different quenching factors for the effective spin gyromagnetic ratio. The obtained theoretical MDM values are compared to different experimentally determined values. On this basis we discuss the possible ways to minimize the discrepancies between the theory and experiment in order to ensure a high accuracy description of ^{229m}Th electromagnetic characteristics. This is of a special importance regarding the current efforts for establishing of a new frequency standard based on ^{229m}Th and referred to as a “nuclear clock”.

1 Introduction

The ^{229}Th nucleus and its exceptionally low-energy 7.8 eV isomeric state ^{229m}Th [1] have attracted much interest in the last decade due to a number of related highly aimed applications such as the so-called “nuclear clock” [2–4], the development of nuclear lasers in the optical range [5] and others [6, 7]. Several recent experimental studies have been focused on the clarification of the isomer decay modes and provided estimates about its life time in charged [8] and neutral [9] electronic states as well as on the magnetic moment of the nucleus in the isomeric state [10].

In our recent theoretical work [11], we have suggested that the energy and electromagnetic characteristics of the ^{229m}Th isomer can be explored through a sophisticated model approach which incorporates the shape-dynamic properties together with the intrinsic structure characteristics typical for the actinide nuclei to which ^{229}Th belongs. The formalism includes a description of the collective quadrupole-octupole vibration-rotation motion (inherent for these nuclei) coupled to the motion of the single (odd) nucleon within a reflection-asymmetric deformed potential with pairing correlations and fully microscopic treatment of the Coriolis interaction. The model approach allows one to determine the energy and radiative decay property of the ^{229m}Th isomer as an integral part of the entire low-lying positive- and negative-parity spectrum and transition probabilities observed in ^{229}Th. On this basis, we have shown that the extremely small isomer energy can be explained as the consequence of a very fine interplay between the rotation-vibration degrees of freedom and the motion of the unpaired neutron. The model calculations predict for the reduced probability $B(M1)$ for magnetic decay of the isomer a value between 0.006 and 0.008 Weisskopf units (W.u.) which is considerably smaller than earlier deduced values of 0.048 W.u. [12, 13] and 0.014 W.u. [14]. This result may explain recently reported experimental difficulties to observe the radiative decay of the isomer [15–17] and suggests a new finer accuracy target for further measurements. At the same time the formalism proposed in [11] provides a reasonable tool to estimate other important characteristics such as the magnetic dipole moment (MDM) which is of a great current interest [10] as a quantity closely related to the electromagnetic decay properties of the isomer. Therefore, in the present article we report first/preliminary model estimations for the MDM in the isomeric as well as in the ground state of ^{229}Th without taking into account the effect of Coriolis mixing in both states. Below we discuss the model conditions under which the obtained MDM values can reach a reasonably good agreement with the corresponding experimental estimates.

In Section 2 we briefly present the model formalism and the way in which the MDM is determined. In Section 3 we give numerical results for the MDMs in the ground and the isomeric state of ^{229}Th together with a relevant discussion based on the comparison with several experimental estimates. In Section 4 concluding remarks are given.

2 Model Approach and Magnetic Dipole Moments

The model Hamiltonian, which corresponds to quadrupole-octupole (QO) vibrations and rotations coupled to the s.p. motion with Coriolis interaction and pairing correlations, can be written in the form [11]

$$H = H_{\text{s.p.}} + H_{\text{pair}} + H_{\text{qo}} + H_{\text{Coriol}} \,. \tag{1}$$

Here $H_{\text{s.p.}}$ is the s.p. Hamiltonian of Deformed Shell Model (DSM) with a Woods-Saxon (WS) potential for axial quadrupole, octupole and higher-multipolarity deformations [18] providing the s.p. energies E^K_{sp} with given value of the projection K of the total and s.p. angular momentum operators $\hat{I}$ and $\hat{j}$, respectively on the intrinsic symmetry axis. H_{pair} is the standard Bardeen-Cooper-Schrieffer (BCS) pairing Hamiltonian [19]. This DSM+BCS part provides the quasi-particle (q.p.) spectrum ϵ^K_{qp} as shown in Ref. [20]. H_{qo} represents oscillations of the even–even core with respect to the quadrupole (β_2) and octupole (β_3) axial deformation variables mixed through a centrifugal (rotation-vibration) interaction [21,22]. $H_{\rm Coriol}$ involves the Coriolis interaction between the even-even core and the unpaired nucleon (see Eq. (3) in [22]). It is treated as a perturbation with respect to the remaining part of (1) and then incorporated into the QO potential of $H_{\rm qo}$ defined for given angular momentum I, parity π and s.p. band-head projection K_b which leads to a joint term [11,23]

$$H_{\rm qo}^{IK_b} = -\frac{\hbar^2}{2B_2}\frac{\partial^2}{\partial\beta_2^2} - \frac{\hbar^2}{2B_3}\frac{\partial^2}{\partial\beta_3^2} + \frac{1}{2}C_2{\beta_2}^2 + \frac{1}{2}C_3{\beta_3}^2 + \frac{\widetilde{X}(I^\pi, K_b)}{d_2\beta_2^2 + d_3\beta_3^2}\,. \tag{2}$$

Here, B_2 (B_3), C_2 (C_3) and d_2 (d_3) are quadrupole (octupole) mass, stiffness and inertia parameters, respectively, and $\widetilde{X}(I^\pi, K_b)$ determines the centrifugal term in which the Coriolis mixing is taken into account (see Eqs. (S1)–(S3) in [24]).

The spectrum of Hamiltonian (1) represents QO vibrations and rotations built on a q.p. state with $K = K_b$ and parity π^b. The corresponding energy expression has the form [11,23]

$$E_{nk}^{\rm tot}(I^\pi, K_b) = \epsilon_{\rm qp}^{K_b} + \hbar\omega\left[2n + 1 + \sqrt{k^2 + b\widetilde{X}(I^\pi, K_b)}\right], \tag{3}$$

where $b = 2B/(\hbar^2 d)$ denotes the reduced inertia parameter and $n = 0, 1, 2, \ldots$ and $k = 1, 2, 3, \ldots$ stand for the radial and angular QO oscillation quantum numbers, respectively, with k odd (even) for the even (odd) parity states of the core [25]. The levels of the total QO core plus particle system, determined by a particular n and $k^{(+)}$ ($k^{(-)}$) for the states with given $I^{\pi=+}$ ($I^{\pi=-}$) form a split (quasi) parity doublet [26]. Furthermore, $\omega = \sqrt{C_2/B_2} = \sqrt{C_3/B_3} \equiv \sqrt{C/B}$ stands for the frequency of the coherent QO mode (CQOM) [21,22] and $d = (d_2 + d_3)/2$.

The Coriolis perturbed wave function corresponding to Hamiltonian (1) with the spectrum (3) is obtained in the first order of perturbation theory and has the form

$$\widetilde{\Psi}_{nkIMK_b}^{\pi,\pi^b} = \frac{1}{\widetilde{N}_{I\pi K_b}}\left[\Psi_{nkIMK_b}^{\pi,\pi^b} + A\sum_{\substack{\nu\neq b\\ (K_\nu = K_b\pm 1, \frac{1}{2})}} C_{K_\nu K_b}^{I\pi}\Psi_{nkIMK_\nu}^{\pi,\pi^b}\right], \tag{4}$$

where the expansion coefficients are given by $C_{K_\nu K_b}^{I\pi} = \widetilde{a}_{K_\nu K_b}^{(\pi\pi^b)}(I)/(\epsilon_{\rm qp}^{K_\nu} - \epsilon_{\rm qp}^{K_b})$ with $\widetilde{a}_{K_\nu K_b}^{(\pi\pi^b)}(I)$ given by Eqs. (S2) and (S3) of [24] and $\widetilde{N}_{I\pi K_b}^2$ is a normalization constant given by Eq. (S5) of [24]. The unperturbed QO core plus particle wave function in Eq. (4) has the form [23]

$$\Psi^{\pi,\pi^b}_{nkIMK}(\eta,\phi,\theta) = \frac{1}{N_K^{(\pi^b)}}\sqrt{\frac{2I+1}{16\pi^2}}\Phi^{\pi\cdot\pi^b}_{nkI}(\eta,\phi)$$
$$\left[D^I_{M\,K}(\theta)\mathcal{F}_K^{(\pi^b)} + \pi\cdot\pi^b(-1)^{I+K}D^I_{M\,-K}(\theta)\mathcal{F}_{-K}^{(\pi^b)}\right], \quad (5)$$

where $D^I_{M\,K}(\theta)$ are the rotation (Wigner) functions, $\Phi^{\pi\cdot\pi^b}_{nkI}(\eta,\phi)$ are the QO vibration functions obtained after solving the Schrödinger equation for the Hamiltonian (2) in radial (η) and angular ϕ coordinates (see [25, 26] for details) and $\mathcal{F}_{K_b}^{(\pi^b)}$ is the parity-projected component of the s.p. wave function of the bandhead state determined by DSM [18]. The quantity

$$N_K^{(\pi^b)} = \left[\left\langle \mathcal{F}_K^{(\pi^b)} \middle| \mathcal{F}_K^{(\pi^b)}\right\rangle\right]^{\frac{1}{2}} \quad (6)$$

is the corresponding parity-projected normalization factor.

Due to the Coriolis interaction the wave function (4) involves a K-mixing of the bandhead s.p. function with other s.p. wave functions. Therefore, states with energies given by Eq. (3) and wave functions determined by (4) with different K_b values appear connected through electromagnetic transitions which otherwise would be suppressed due to the axial symmetry of the system. On this basis we developed the model formalism for calculation of reduced $B(E1)$, $B(E2)$, $B(E3)$ and $B(M1)$ transition probabilities for the energy spectrum (3) (see [24] for the explicit expressions).

To estimate the magnetic moments in ^{229}Th in relation to the spectroscopic description obtained in the above CQOM-DSM-BCS framework in the present work we apply a simple approach involving the s.p. wave functions without taking into account the Coriolis mixing. Thus, we consider that the magnetic moment in a rotation state built on given bandhead quasiparticle configuration with given K-value can be determined as [19]

$$\mu = \mu_N\left[g_R\frac{I(I+1)-K^2}{I+1} + g_K\frac{K^2}{I+1}\right], \quad (7)$$

with $\mu_N = e\hbar/(2mc)$, $g_R = Z/A$ and

$$g_K = \frac{1}{K}\langle\mathcal{F}_K|g_s\cdot\Sigma + g_l\cdot\Lambda|\mathcal{F}_K\rangle, \quad (8)$$

where Σ and Λ (with $\Sigma+\Lambda = K$) are the intrinsic spin and orbital angular momentum projections, respectively, and g_l and g_s are the standard gyromagnetic ratios. The proton and neutron g_s values are attenuated by a commonly used quenching factor q between 0.6 and 0.7 compared to the free values.

However in the present case we have to necessarily take into account the presence of the reflection asymmetry in the problem. Therefore in (8) we take the parity projected component of the s.p. wave function $\mathcal{F}_K \to \mathcal{F}_K^{(\pi^b)}/N_K^{(\pi^b)}$ with $N_K^{(\pi^b)}$ given by (6). Then we have

$$g_K^{(\pi^b)} = \frac{1}{K}\frac{1}{[N_K^{(\pi^b)}]^2}\langle\mathcal{F}_K^{(\pi^b)}|g_s\cdot\Sigma + g_l\cdot\Lambda|\mathcal{F}_K^{(\pi^b)}\rangle. \tag{9}$$

It should be noted that the complete treatment of nuclear MDM properties within our CQOM-DSM-BCS approach requires to take into account the Coriolis mixing effect as included in the full model function (4). By recognizing that such a study is mandatory for a subsequent work we remark that the simplified approach to MDM in the present work could serve as a first step allowing eventual comparisons with other model approaches without Coriolis interaction as well as a basis for estimating the role of the Coriolis mixing after being taken into account.

3 Magnetic Moment in ^{229}Th

In [11] we applied the above CQOM-DSM approach to the low-lying part of the experimental ^{229}Th spectrum [27] including positive- and negative-parity levels with energy below 400 keV as shown in Fig. 1 of Ref. [11]. The spectrum was obtained in the form of an yrast quasi parity-doublet (QPD) built on the 5/2[633] ground-state (g.s.) s.p. orbital and non-yrast QPD built on the 3/2[631] orbital corresponding to the $3/2^+$ isomeric state. All model parameters, quadrupole (β_2) and octupole (β_3) deformations entering DSM, the BCS pairing parameters, the collective CQOM parameters and the Coriolis mixing strength were determined so that both states $5/2^+$ g.s. and the isomeric $3/2^+$ were obtained as a quasi-degenerate pair, with the latter taking values in the range of the experimental one, while the excited QPD levels and the available experimental B(E2) and B(M1) values [28] were reproduced reasonably well. On this basis we have made predictions for the M1 and E2 decay probabilities for the $3/2^+$ isomer state.

In the present work we calculated the magnetic moment in the ground and isomeric state of ^{229}Th corresponding to the parameters of the above mentioned model description. As for the magnetic moment the important ingredient is the s.p. wave function and the quenching of the spin gyromagnetic factor we remark that the former is determined in DSM for $\beta_2 = 0.240$ and $\beta_3 = 0.115$ while for the g_s quenching factor we take two different values $q = 0.6$ used in the calculation of B(M1) values in [11] as well in the calculation of MDM in high-K isomers [20] and $q = 0.7$ commonly used in other works [19].

The result of the present MDM calculations is shown in Table 1 in comparison with several available values obtained from earlier calculations and hyperfine splitting measurements. An earlier calculation for the isomeric MDM based on the usual Nilsson model provided the value of $\mu_{\text{IS}} = -0.076\ \mu_N$ [12]. The g.s. MDM was extracted from an earlier atomic hyperfine splitting experiment [29] yielding the value $\mu_{\text{GS}} = 0.46(4)\ \mu_N$. This value was corrected in

Table 1. Theoretical MDM values (in magneton units μ_N) obtained in this work given in comparison with other calculations and experimental values.

μ_{state}	This work $q{=}0.6$	This work $q{=}0.7$	Ref. [12]	Ref. [29]	Ref. [30]	Ref. [32]	Ref. [10]
μ_{GS}	0.677	0.743	–	0.46(4)	0.360(7)	–	–
μ_{IS}	-0.253	-0.334	-0.076	–	–	-0.30 - -0.38	$-0.37(6)$

Ref. [30] to $\mu_{\text{GS}} = 0.360(7)$ μ_N based on a more recent measurement of the hyperfine structure of ^{229}Th^{3+} ions [31]. The first experimental observation of the isomer hyperfine splitting in ^{229}Th^{2+} was reported only recently [10]. Based on this measurement, an isomer MDM value of $\mu_{\text{IS}} = -0.37(6)$ [10] or in the range of between -0.30 and -0.38 μ_N [32] were extracted.

As seen from Table 1 we have obtained for the ground state MDM the following two values, $\mu_{\text{GS}} = 0.677$ μ_N for g_s quenching factor $q = 0.6$ and $\mu_{\text{GS}} = 0.743$ μ_N for $q = 0.7$. Comparing them to the values in [29] and [30] we see that they overestimate the latter by a factor between 1.5 and 2. On the other hand our values for the isomer MDM $\mu_{\text{IS}} = -0.253$ μ_N for $q = 0.6$ and $\mu_{\text{IS}} = -0.334$ μ_N for $q = 0.7$ corroborate the values in Refs. [32] and [10]. We see that the second value even enters the error bar for the value of $\mu_{\text{IS}} = -0.37(6)$ μ_N in [10]. We emphasize that our values for the MDMs in ^{229}Th are not obtained through a separate fit but correspond to the model parameters determined in the energy and B(M1), B(E2) fit from which the spectrum in Fig. 1 of Ref. [11] is obtained. This includes the spin gyromagnetic quenching $q = 0.6$ for which the obtained MDM values correspond to the theoretical B(M1) values denoted by "Th1" in Table 1 of [11]. (Note that only the B(M1) values depend on q whereas the B(E2)s and the energy not.) Thus, for this particular quenching factor we have $B(M1; 3/2^+_{\text{IS}} \to 5/2^+_{\text{GS}}) = 0.008$ W.u. predicted for the isomer M1 decay. For the larger $q = 0.7$ the model calculation with the all other parameters being the same gives $B(M1; 3/2^+_{\text{IS}} \to 5/2^+_{\text{GS}}) = 0.009$ W.u. Therefore, we see that the MDM values obtained in the present work are firmly related with the model predictions for the M1 decay mode of the ^{229m}Th isomer. This result suggests that further refinements of the model parameters providing better description of ^{229}Th MDMs in particular the g.s. MDM value would be of use to achieve higher predictive value of the approach in the study of the 7.8 eV isomer-decay properties. As mentioned in the end of previous Sec. 2 in this case the Coriolis mixing should be necessarily taken into account in the MDM calculation.

4 Conclusion

In conclusion, we have shown that the CQOM-DSM-BCS model description of the QPD spectrum and $B(M1)$ and $B(E2)$ transition rates in ^{229}Th provides a possibility for reasonable description of the MDM in the isomeric state. The result for the g.s. MDM suggests that further refinements of the approach including the Coriolis mixing are needed to achieve better agreement with the experimental data. On the other hand the model predicted MDM values may suggest in turn possible correction in the experimental values and provide a direction for further experimental measurements. Therefore, the future activity from both sides, theory and experiment, would be of a great importance for the revealing in detail the electromagnetic properties of the nucleus ^{229}Th as well as for clarifying the dynamical mechanism which governs the radiative decay of its 7.8 eV isomeric state.

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References

[1] B. R. Beck et al., *Phys. Rev. Lett.* **98** (2007) 142501; LLNL-PROC-415170 (2009).
[2] C. J. Campbell et al., *Phys. Rev. Lett.* **108** (2012) 120802.
[3] E. Peik and C. Tamm, *Europhys. Lett.* **61** (2003) 181.
[4] E. Peik and M. Okhapkin, *C. R. Phys.* **16** (2015) 516.
[5] E. V. Tkalya, *Phys. Rev. Lett.* **106** (2011) 162501.
[6] T. Bürvenich et al., *Phys. Rev. Lett.* **96** (2006) 142501.
[7] V. V. Flambaum, *Phys. Rev. Lett.* **97** (2006) 092502.
[8] L. von der Wense et al., *Nature (London)* **533** (2016) 47.
[9] B. Seiferle, L. von der Wense and P. G. Thirolf, *Phys. Rev. Lett.* **118** (2017) 042501.
[10] J. Thielking, M. V. Okhapkin, P. Glowacki, D. M. Meier, L. von der Wense, B. Seiferle, C. E. Düllmann, P. G. Thirolf and E. Peik, *Nature (London)* **556** (2018) 321.
[11] N. Minkov and A. Pálffy, *Phys. Rev. Lett.* **118** (2017) 212501.
[12] A. M. Dykhne and E. V. Tkalya, *JETP Lett.* **67** (1998) 251.
[13] E. V. Tkalya, C. Schneider, J. Jeet and E. R. Hudson, *Phys. Rev. C* **92** (2015) 054324.
[14] E. Ruchowska et al., *Phys. Rev. C* **73** (2006) 044326.
[15] J. Jeet et al., *Phys. Rev. Lett.* **114** (2015) 253001.
[16] A. Yamaguchi et al., *New J. Phys.* **17** (2015) 053053.
[17] L. von der Wense, *On the direct detection of $^{229\mathrm{m}}$Th*, PhD Thesis, Ludwig Maximilian University Munich (2016).
[18] S. Cwiok, J. Dudek, W. Nazarewicz, J. Skalski and T. Werner, *Comp. Phys. Comm.* **46** (1987) 379.

[19] P. Ring and P. Schuck, *The Nuclear Many-Body Problem*, (Springer, Heidelberg, 1980).

[20] P. M. Walker and N. Minkov, *Phys. Lett. B* **694** (2010) 119.

[21] N. Minkov, P. Yotov, S. Drenska, W. Scheid, D. Bonatsos, D. Lenis and D. Petrellis, *Phys. Rev. C* **73** (2006) 044315.

[22] N. Minkov, S. Drenska, P. Yotov, S. Lalkovski, D. Bonatsos and W. Scheid, *Phys. Rev. C* **76** (2007) 034324.

[23] N. Minkov, *Physica Scripta* **T154** (2013) 014017.

[24] see Supplemental Material at [https://journals.aps.org/prl/abstract/10.1103/PhysRevLett.118.212501#supplemental] for complete analytical expressions and additional details of the formalism.

[25] N. Minkov, S. Drenska, M. Strecker, W. Scheid and H. Lenske, *Phys. Rev. C* **85** (2012) 034306.

[26] N. Minkov, S. Drenska, K. Drumev, M. Strecker, H. Lenske and W. Scheid, *Phys. Rev. C* **88** (2013) 064310.

[27] http://www.nndc.bnl.gov/ensdf/.

[28] http://www.nndc.bnl.gov/nudat2/indx_adopted.jsp.

[29] S. Gerstenkorn et al., *J. Phys. (Paris)* **35** (1974) 483.

[30] M. S. Safronova, U. I. Safronova, A. G. Radnaev, C. J. Campbell and A. Kuzmich, *Phys. Rev. A* **88** (2013) 060501(R).

[31] C. J. Campbell, A. G. Radnaev and A. Kuzmich, *Phys. Rev. Lett.* **106** (2011) 223001.

[32] R. Müller et al., *Phys. Rev. A* **98** (2018) 020503(R).