THE MAGNETIC MOMENT AS A CONSTRAINT IN DETERMINING THE ^{229m}Th ISOMER DECAY RATES*

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Dedicated to the memory of Professor Adam Sobiczewski

Recently, the magnetic and electric radiative decay rates of the 7.8 eV ^{229m}Th isomer have been predicted within a model of nuclear collective quadrupole–octupole (QO) and single particle (s.p.) motions with the Coriolis interaction. As a next step, in the study we examine the magnetic dipole moment (MDM) in the $K=5/2^+$ ground and $K=3/2^+$ isomeric states based on the parity-projected s.p. wave functions obtained for the odd neutron in both states without consideration of the Coriolis mixing effects. The comparison with experimental data shows that the description of MDMs may impose additional constraint on the model parameters providing further tuning of the predicted isomer-decay rates in favour of the efforts for establishing of a "nuclear clock" frequency standard.

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1. Introduction

In the recent years, the nucleus ^{229}Th has attracted much interest due to its extremely low-energy 7.8 eV isomeric state [1] which is expected to allow a number of challenging applications such as the elaboration of a "nuclear

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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 life time [8, 9], and the MDM of the nucleus in the isomeric state as well [10, 11].

In our recent theoretical work [12], we have suggested that the energy and electromagnetic characteristics of the ^{229m}Th isomer can be clarified within nuclear model approach describing the shape-dynamics and intrinsic structure properties typical for the actinide region to which ^{229}Th belongs. The model describes the QO vibration–rotation motion (inherent for the nuclei of this region) coupled through the Coriolis interaction to the motion of the odd nucleon in a reflection-asymmetric deformed potential with pairing correlations. The approach allowed us to determine the energy and radiative decay property of the ^{229m}Th isomer as a part of the entire low-lying 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 [12]. The model calculations predict for the reduced probability $B(\mathrm{M1})$ for magnetic decay of the isomer a value in the range of 0.006–0.008 W.u. which is considerably smaller than earlier deduced values of 0.048 W.u. [13, 14] and 0.014 W.u. [15]. This result explains the current difficulties in observing experimentally the radiative decay of the isomer [16–18] and suggests a new finer accuracy goal for further measurements.

At the same time, it motivates us to extend the study of [12] by considering the MDM as a quantity closely related to the electromagnetic decay properties of the isomer. Further strong motivation is given by the just appearing experimental data on the isomer MDM [10, 11] which obviously need an adequate theoretical explanation. Therefore, in the present article, we report on model estimations for the MDM in the isomeric and ground state of ^{229}Th made on the basis of the model solution for the energy spectrum and transition rates obtained in [12]. In this work, we do not take into account the effect of Coriolis mixing in both states. Below, it will be seen that the comparison with the experimental data on MDM may provide an additional constraint on the conditions under which the $B(\mathrm{M1})$ and $B(\mathrm{E2})$ isomer-decay rates are calculated increasing in this way the reliability of the model predictions.

In Sec. 2, we briefly present the model formalism and the way in which the MDM is determined. In Sec. 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 Sec. 4, concluding remarks are given.

2. Model approach and magnetic dipole moments

The Hamiltonian of QO vibrations and rotations coupled to the s.p. motion with the Coriolis interaction and pairing correlations, has the form [12] of

$$H = H_{\rm sp} + H_{\rm pair} + H_{\rm qo} + H_{\rm Coriol}\,. \tag{1}$$

Here, $H_{\rm sp}$ is the s.p. Hamiltonian of Deformed Shell Model (DSM) with a Woods–Saxon (WS) potential for axial quadrupole, octupole and higher-multipolarity deformations [19] providing the s.p. energies $E^K_{\rm sp}$ 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. $H_{\rm pair}$ is the standard Bardeen–Cooper–Schrieffer (BCS) pairing Hamiltonian [20]. This DSM+BCS part provides the quasi-particle (q.p.) spectrum $\epsilon^K_{\rm qp}$ as shown in Ref. [21]. $H_{\rm qo}$ 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 [22–25]. $H_{\rm Coriol}$ involves the Coriolis interaction between the even–even core and the unpaired nucleon (see Eq. (3) in [23]). 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 [12, 26]

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

Here, B_2 (B_3), C_2 (C_3) and d_2 (d_3) are quadrupole (octupole) mass, stiffness and inertia parameters, respectively, and $\widetilde{X}(I^\pi,K_b)$ is a centrifugal term with the Coriolis interaction (see Eqs. (S1)–(S3) in [27]).

The spectrum of Hamiltonian (1) represents QO vibrations and rotations built on a q.p. state with $K=K_b$ and parity π^b and has the form [12, 26] of

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

where b is an inertia parameter, $n=0,1,2,\ldots$ and $k=1,2,3,\ldots$ are the QO oscillation quantum numbers which determine a quasi-parity-doublet (QPD) structure of the spectrum [25] and $\omega=\sqrt{C_2/B_2}=\sqrt{C_3/B_3}\equiv\sqrt{C/B}$ is the frequency of the coherent QO mode (CQOM) originally assumed in [22].

The Coriolis perturbed wave function corresponding to Hamiltonian (1) with spectrum (3) is obtained in the form of

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

where the expansion coefficients are given by $C^{I\pi}_{K_\nu K_b} = \widetilde{a}^{(\pi\pi^b)}_{K_\nu K_b}(I)/(\epsilon^{K_\nu}_{\rm qp} - \epsilon^{K_b}_{\rm qp})$ with $\widetilde{a}^{(\pi\pi^b)}_{K_\nu K_b}(I)$ given by Eqs. (S2) and (S3) of [27] and $\widetilde{N}^2_{I\pi K_b}$ is a normalization constant given by Eq. (S5) of [27]. The unperturbed QO core plus particle wave function in Eq. (4) has the form [25, 26] of

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

where $D^I_{MK}(\theta)$ are the rotation functions, $\Phi^{\pi\,\pi^b}_{nkI}(\eta,\phi)$ are the QO vibration functions in radial (η) and angular ϕ coordinates (see [24, 25] for details), and $\mathcal{F}^{(\pi^b)}_{K_b}$ is the parity-projected component of the s.p. wave function of the band-head state determined by DSM [19] with $N^{(\pi^b)}_K = \left[\left\langle \mathcal{F}^{(\pi^b)}_K \middle| \mathcal{F}^{(\pi^b)}_K \right\rangle \right]^{\frac{1}{2}}$ being the corresponding parity-projected normalization factor.

The Coriolis perturbed wave function (4) involves a K-mixing of the band-head s.p. wave function with other s.p. functions thus allowing the transitions between QPD states with different K_b values which are otherwise suppressed due to the axial symmetry. (Expressions for the relevant B(E1), B(E2), B(E3) and B(M1) transition probabilities are given in [27].)

To make simple estimates for the MDM of ^{229m}Th corresponding to the spectroscopic description obtained in the above CQOM-DSM-BCS model, we consider the parity-projected s.p. wave functions without taking into account the Coriolis mixing. Then the MDM in a rotation state built on a band-head q.p. configuration with given K_b-value is determined as [20]

$$\mu = \mu_N \left[g_R \frac{I(I+1) - K_b^2}{I+1} + g_{K_b} \frac{K_b^2}{I+1} \right] , \quad (6)$$

where $\mu_N = e\hbar/(2mc)$, g_R is the collective gyromagnetic factor which can be taken in a rough approximation as $g_R = Z/(N+Z)$ and

$$
\begin{aligned}
g_{K_b} &= \frac{1}{K_b}\left\langle \tilde{\mathcal{F}}_{K_b} \middle| g_s\,\Sigma + g_l\,\Lambda \middle| \tilde{\mathcal{F}}_{K_b} \right\rangle \\
&= \frac{1}{K_b}\frac{1}{\left[N_K^{(\pi^b)}\right]^2}\left\langle \mathcal{F}_{K_b}^{(\pi^b)} \middle| g_s\,\Sigma + g_l\,\Lambda \middle| \mathcal{F}_{K_b}^{(\pi^b)} \right\rangle \qquad (7)
\end{aligned}
$$

is the intrinsic gyromagnetic factor determined through the parity-projected and renormalized s.p. wave function of the band-head state $\tilde{\mathcal{F}}_{K_b} = \mathcal{F}_{K_b}^{(\pi^b)}/N_K^{(\pi^b)}$ with $N_K^{(\pi^b)}$ given below Eq. (5). Here, 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 orbital and spin gyromagnetic factors, respectively. The g_s values are attenuated with respect to the free-nucleon values by a quenching factor q, which can be taken between 0.6 and 0.7.

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

3. Numerical results for the MDM in ^{229}Th

We calculate the MDM in the ground and isomeric state of ^{229}Th obtained in the solution of the CQOM-DSM-BCS model for the low-lying QPDs of this nucleus (see Fig. 1 in [12]). The spectrum is obtained in the form of an yrast QPD built on the 5/2[633] ground-state (g.s.) orbital and non-yrast QPD built on the 3/2[631] orbital corresponding to the isomeric state. The model parameters are determined so that both band-head states appear as a quasi-degenerate pair. The important ingredient for the calculation of MDM is the parity-projected s.p. wave function which enters g_{K_b} in (7). We take it as determined in [12] for $\beta_2 = 0.240$ and $\beta_3 = 0.115$. For the quenching of the spin gyromagnetic factor g_s, we take two different values: $q = 0.6$, used in the calculation of the B(M1) transition rates in [12] as well as in the calculation of MDM in high-K isomers [21], and $q = 0.7$ used by other authors [20]. Thus, we obtain two different predictions for the g.s. and isomer MDMs with corresponding different predictions for the $B(\mathrm{M1})_{\mathrm{IS}} \to \mathrm{GS}$ isomer-decay probability.

The result is shown in Table I in comparison with several available values obtained from earlier calculations and atomic-state hyperfine splitting measurements. An earlier calculation for the isomeric MDM based on the usual

Nilsson model provides the value of $\mu_{\rm IS} = -0.076\,\mu_N$ [13]. The g.s. MDM was extracted from an earlier atomic hyperfine splitting experiment [28] yielding the value $\mu_{\rm GS} = 0.46(4)\,\mu_N$. This value was corrected in Ref. [29] to $\mu_{\rm GS} = 0.360(7)\,\mu_N$ based on a more recent measurement of the hyperfine structure of $^{229}{\rm Th}^{3+}$ ions [30]. The first experimental observation of the isomer hyperfine splitting in $^{229}{\rm Th}^{2+}$ was reported only recently [10]. Based on this measurement, an isomer MDM value of $\mu_{\rm IS} = -0.37(6)$ [10] or in the range of between -0.30 and $-0.38\,\mu_N$ [11] were extracted.

TABLE I

Theoretical MDM values (in magneton units μ_N) obtained for two g_s quenching factors $q = 0.6$ and 0.7 are given in comparison with other calculation and experimental values. The corresponding predicted $B({\rm M1})_{\rm IS} \to {\rm GS}$ values (in W.u.) for a transition from the isomer to the g.s. are also given.

$\mu_{\rm state}$ and B(M1)	This work $q = 0.6$	$q = 0.7$	Reference [13]	[28]	[29]	[11]	[10]
$\mu_{\rm GS}$	0.677	0.743	—	0.46(4)	0.360(7)	—	—
$\mu_{\rm IS}$	−0.253	−0.334	−0.076	—	—	$-0.30 \div -0.38$	−0.37(6)
$B({\rm M1})_{\rm IS} \to {\rm GS}$	0.008	0.009					

As seen from Table I, we have obtained for the ground state MDM the following two values, $\mu_{\rm GS} = 0.677\,\mu_N$ for g_s quenching factor $q = 0.6$ and $\mu_{\rm GS} = 0.743\,\mu_N$ for $q = 0.7$. Comparing them to the values in [28] and [29], 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 $\mu_{\rm IS} = -0.253\,\mu_N$ for $q = 0.6$ and $\mu_{\rm IS} = -0.334\,\mu_N$ for $q = 0.7$ corroborate the values in Refs. [10] and [11]. We see that the second value enters the error bar for the value of $\mu_{\rm IS} = -0.37(6)\,\mu_N$ in [10] though the corresponding $\mu_{\rm GS}$ value is less favoured by the experiment. 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. [12] is obtained. This includes the spin gyromagnetic quenching $q = 0.6$ used for the calculations in Ref. [12]. (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 $B({\rm M1}; 3/2^+_{\rm IS} \to 5/2^+_{\rm GS}) = 0.008$ 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 $B({\rm M1}; 3/2^+_{\rm IS} \to 5/2^+_{\rm GS}) = 0.009$ W.u. Therefore, we see that the MDM values obtained in the present work are firmly related with the model predictions [12] 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, may constrain the predictions for the B(M1) transition rates. In such a way, the involvement of the MDM in the study would raise the predictive value of the approach in the clarification of the 7.8 eV isomer-decay properties. However, as mentioned at the end of Sec. 2, for the implementation of this task, the Coriolis mixing should be necessarily taken into account.

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. In this way, the description of the MDMs appears as an additional constraint on the determination of the isomer-decay probabilities predicted by the model. On the other hand, the model-predicted MDM values may, in turn, suggest a 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 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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