

Anomalous magnetic hyperfine structure of the ^{229}Th ground-state doublet in muonic atoms

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The magnetic hyperfine (MHF) splitting of the ground and low-energy $3/2^+$ (7.8 ± 0.5 eV) levels in the ^{229}Th nucleus in the muonic atom $(\mu_{1S_{1/2}}^-)^{229}\text{Th}^*$ is calculated considering the distribution of the nuclear magnetization in the framework of the collective nuclear model with wave functions of the Nilsson model for the unpaired neutron. It is shown that (a) deviation of the MHF structure of the isomeric state exceeds 100% from its value for a pointlike nuclear magnetic dipole (the order of sublevels is reversed); (b) partial inversion of levels of the ^{229}Th ground-state doublet and spontaneous decay of the ground state to the isomeric state occur; (c) the $E0$ transition, which is sensitive to differences in the mean-square charge radii of the doublet states, is possible between mixed sublevels with $F = 2$; and (d) MHF splitting of the $3/2^+$ isomeric state may be in the optical range for certain values of the intrinsic g_K factor and a reduced probability of a nuclear transition between the isomeric and the ground states.

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Introduction. The unique transition between the low-lying isomeric level $3/2^+$ ($E_{is} = 7.8 \pm 0.5$ eV) (its energy is measured in [1] and its existence is confirmed in [2]) and the ground $5/2^+$ (0.0) state in the ^{229}Th nucleus draws the attention of specialists from different areas of physics. The reason is the anomalous low energy of the transition. Its proximity to the optical range gives us hope for a number of scientific breakthroughs that could have a significant impact on technological development and applications, such as a metrological standard for time [3–5] and a laser at the nuclear transition in the vacuum ultraviolet (VUV) range [6]. The relative effect of the variation of the fine-structure constant e^2 (we use the system of units $\hbar = c = 1$) and the strong interaction parameter m_q/Λ_{QCD} [7] are also of considerable scientific interest. Finally, we mention the decay of the isomeric nuclear level via the electronic bridge [8], high sensitivity of the nuclear transition to the chemical environment, and ability to use the thorium isomer as a probe to study the physicochemical properties of solids [8], cooperative spontaneous Dicke emission [9] in the system of excited nuclei ^{229}Th , and accelerated α decay of the ^{229}Th nucleus via the isomeric state [10]. The behavior of the excited ^{229}Th nucleus inside dielectrics with a large band gap is of particular interest [11]. Since there is no conversion decay channel in such a dielectric, the nucleus can absorb and emit VUV-range photons directly, without interaction with the electron shell [10]. As a result, studying the isomeric state by optical methods becomes possible [5, 12–15].

In this work the ^{229}Th ground-state doublet is investigated in the muonic atom $(\mu_{1S_{1/2}}^-)^{229}\text{Th}^*$. The muon on the $1S_{1/2}$ atomic orbit creates a very strong magnetic field at the nucleus [16, 17]. The interaction of this field with the magnetic moments of nuclear states leads to a magnetic hyperfine (MHF) splitting of nuclear levels (see, for example, [18–28], and references therein). We demonstrate here that the MHF splitting has a

number of nontrivial features in the case of $(\mu_{1S_{1/2}}^-)^{229}\text{Th}^*$: the partial inversion of nuclear sublevels and spontaneous decay of the ground state $5/2^+$ to the isomeric $3/2^+$ state, the anomaly deviation of the MHF structure of the isomeric state from its value for a pointlike nucleus, the important role of the dynamic effect of finite nuclear size (or the penetration effect) in the state mixing, the possible existence of the electric monopole transition and optical transitions between MHF sublevels, etc. This situation is very unusual and looks promising with regard to experimental research.

The Fermi contact interaction. Let us consider the system $(\mu_{1S_{1/2}}^-)^{229}\text{Th}^*$, which consists of a muon bound on the $1S_{1/2}$ shell of a muonic atom and the ^{229}Th nucleus. The muon in the $(1S_{1/2})^1$ state results in a strong magnetic field in the center of the ^{229}Th nucleus. The value of this field is given by the formula for the Fermi contact interaction,

$$\mathbf{H}_\mu = -\frac{16\pi}{3} \frac{m_e}{m_\mu} \mu_B \frac{\boldsymbol{\sigma}}{2} |\psi_\mu(0)|^2, \quad (1)$$

where m_e and m_μ are the masses of the electron and muon, respectively, $\mu_B = e/2m_e$ is the Bohr magneton, $\boldsymbol{\sigma}$ are the Pauli matrices, and $\psi_\mu(0)$ is the amplitude of the muon Dirac wave function at the origin.

The amplitude $\psi_\mu(0)$ can be calculated numerically by solving the Dirac equations for the radial parts of the large, $g(x)$, and small, $f(x)$, components of $\psi_\mu(x)$:

$$\begin{aligned} xg'(x) - b[E + 1 - V(x)]xf(x) &= 0, \\ xf'(x) + 2f(x) + b[E - 1 - V(x)]xg(x) &= 0. \end{aligned}$$

Here $x = r/R_0$, where r is the muon coordinate in the spherical coordinate system and $R_0 = 1.2A^{1/3}$ fm is the average radius of the ^{229}Th nucleus, which has the form of a charged sphere, $b = m_\mu R_0$, and E and $V(x)$ are, respectively, the muon binding and potential energies (in the units of m_μ) in the field produced by the nucleus protons. (For lower muonic states, electron screening plays a negligible role [18, 27]. Therefore we neglect

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Here, $E_0 = -2e^2 M_p / [3(M_p R_0)^2]$, g_K is the intrinsic g factor, $\rho_n(\mathbf{y}) = \varphi_K(\mathbf{y})^* \varphi_K(\mathbf{y})$, $\mathbf{y} = \mathbf{R}/R_0$, $\Theta(I, \theta) = \sqrt{4\pi/5Y_{20}(\theta)(2I+1)/[I(2I+3)]}$. The first term in square brackets in Eq. (5), $\langle \mathcal{M} \rangle = \int_0^\infty f(x)g(x)dx = -0.1895$, corresponds to the interaction of the muon with a point nuclear magnetic dipole. The resulting energy sublevels are close to the values calculated with Eq. (1).

For the unpaired neutron the wave functions φ_K were taken from the Nilsson model. The structure of the intrinsic state φ_K of the ^{229}Th ground state $5/2^+(0.0)$ is $K^\pi[Nn_z\Lambda] = 5/2^+[633]$. The structure of the isomeric state $3/2^+(7.8 \text{ eV})$ is $3/2^+[631]$ [33]. For each of these states, the wave function has the form $\varphi_K = \phi_\Lambda(\varphi)\phi_{\Lambda,n_r}(\eta)\phi_{n_z}(\zeta)$, where the quantum number $n_r = (N - n_z - \Lambda)/2$, the variables on the axes $\zeta = R_0\sqrt{M_p\omega_z}y\cos\theta$, $\eta = R_0\sqrt{M_p\omega_\perp}y\sin\theta$, the energies of the oscillatory quanta $\omega_z = \omega_0\sqrt{1+2\delta/3}$ and $\omega_\perp = \omega_0\sqrt{1-4\delta/3}$, where $\omega_0 = 41/A^{1/3}$ MeV is the harmonic oscillator frequency, $\delta = 0.95\beta$, and β is the parameter of the deformation of the nucleus defined in terms of the expansion of the radius parameter $R = R_0(1 + \beta Y_{20}(\theta) + \dots)$.

The constituent wave functions are as follows: $\phi_\Lambda(\varphi) = e^{i\Lambda\varphi}/\sqrt{2\pi}$, $\phi_{\Lambda,n_r}(\eta) = e^{-\eta^2/2}\eta^\Lambda L_{n_r}^{(\Lambda)}(\eta^2)/N_{\eta_r}$, $\phi_{n_z}(\zeta) = e^{-\zeta^2/2}H_{n_z}(\zeta)/N_{\zeta}$, where $L_{n_r}^{(\Lambda)}$ is the generalized Laguerre polynomial, H_{n_z} is the Hermite polynomial [34], and $N_{\eta_r, \zeta}$ are the normalization factors. The density distributions of the unpaired neutron in states $5/2^+[633]$ and $3/2^+[631]$ averaged over the angles θ and φ are shown in Fig. 1. In our numerical calculations we took into account the asymmetry of the nucleon wave functions in Eq. (5) but neglected the small difference between ω_z and ω_\perp .

For the core magnetization we used the classical density of the magnetic moment, $\rho_c^m \propto x^2/\{1 + \exp[(x-1)/\chi]\}$, obtained from proton density ρ_p by averaging over the angles. This quadratic dependence was used in [19] and [35]. The normalized function ρ_c^m is shown in Fig. 1.

The resulting scheme of MHF splitting for $(\mu_{15/2}^{229}\text{Th})^*$ is shown in Fig. 2. For g factors of the ground state we have used values which are accepted nowadays: $g_R = 0.309$, $g_K = 0.128$ [36]. The reduction of the MHF structure in comparison with the model of the point nuclear magnetic dipole is about 56% for the $5/2^+(0.0)$ state.

For calculation of the isomeric state we have taken $g_R = 0.309$ and $g_K = -0.29$ [37], which is obtained from the mean value $|g_K - g_R| = 0.60$ (the values $|g_K - g_R| = 0.59 \pm 0.14$ and 0.61 ± 0.10 were measured in [38]). The gyromagnetic ratio $g_R = 0.309 \pm 0.016$ from [36] is determined with a much higher precision than $|g_K - g_R|$ for band $3/2^+[631]$, and the existing uncertainty in $|g_K - g_R|$ is related exclusively to g_K : $g_K = 0.29 \pm 0.12$. This leads to uncertainty in the position of levels (see Fig. 2).

A somewhat paradoxical situation can take place because of the complex structure of the magnetic moment of the isomeric state and the behavior of the muon wave function (currently we consider a variant without mixing of states with equal values of F). From Fig. 3 it follows that in the range $-0.30 < g_K < -0.29$ the $3/2^+[631]$ state has a nonzero magnetic moment, whereas MHF splitting is absent or very weak. Conversely, the magnetic moment of the isomeric level equals 0 for $g_K \approx -0.206$, while the MHF splitting is relatively large. The reason

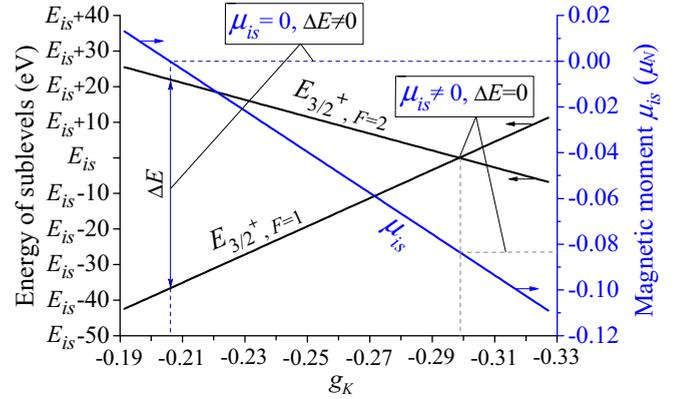


FIG. 3. Imbalance of the MHF interaction for the composed magnetic moment of the isomeric state in ^{229}Th : energies of the sublevels relative to E_{is} and the magnetic moment μ_{is} as a function of the gyromagnetic factor g_K in the absence of mixing of the states with $F = 2$ (see text for details).

is the following. The magnetic field generated by the spin of the nucleon is sensitive to the nonsphericity of the wave functions φ_K . This leads to the appearance of the additional factor $\Theta(I, \theta)$ in the spin part of Eq. (5) [30,31]. Averaging over the angles reduces the spin contribution with respect to the orbital part. A small imbalance emerging in the system leads to violation of the “fine-tuning” between the spin and the orbital parts of the magnetic moment and to the effect described above. This mechanism can also occur in other nuclei with low energy (up to some kiloelectronvolts) levels.

Mixing of sublevels with $F = 2$. To find the final position of the sublevels we now consider the mixing of states with $F = 2$ [25]. The interaction energy, \mathcal{E} , of the nuclear and muon currents during the transition between the $|3/2^+, F = 2\rangle$ sublevel with energy E_1 and the $|5/2^+, F = 2\rangle$ sublevel with energy E_2 can be found from equations given in Refs. [39] and [40]. They generalize the static Bohr-Weisskopf effect for the case of nuclear excitation at the electron (muon) transitions in the atomic shell. For the $M1$ transition we obtain

$$\mathcal{E} = E_0 \xi \langle \mathcal{M} \rangle \sqrt{(15/2) B_{W.u.}(M1; 3/2^+ \rightarrow 5/2^+)},$$

where $B_{W.u.}(M1; 3/2^+ \rightarrow 5/2^+) = 3.0 \times 10^{-2}$ is the reduced probability of the nuclear isomeric transition in Weisskopf’s units [41], and ξ is a factor that takes into account the dynamic effect of the nuclear size [40] or the penetration effect [42]. Calculation of the nuclear current with the neutron wave function in the Nilsson model gives the value of $\xi = 0.45$. As a result, we have $\mathcal{E} \simeq 150 \text{ eV}$.

The energies of the new sublevels with $F = 2$ are calculated according to the formulas [43]

$$E_{1,2'} = [E_1 + E_2 \pm \sqrt{(E_1 - E_2)^2 + (2\mathcal{E})^2}]/2,$$

where $E_{1(2')}$ are the energies of the new sublevels $|3/2^+(5/2^+), F = 2\rangle'$. We emphasize that these energies are valid for the most probable values of g_K and $B_{W.u.}(M1; 3/2^+ \rightarrow 5/2^+)$. Variations of the parameter g_K in the range $(g_K = 0.29 \pm 0.12)$ and the reduced probability of the nuclear transition (currently $3 \times 10^{-3} \leq B_{W.u.}(M1; 3/2^+ \rightarrow 5/2^+) \leq 5 \times 10^{-2}$ [41]) gives a fairly

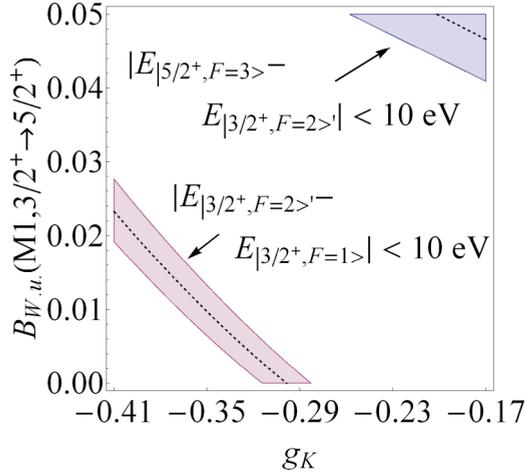


FIG. 4. Range of values of g_K and $B_{W.u.}(M1; 3/2^+ \rightarrow 5/2^+)$ at which the transitions between the sublevels lie in the optical or VUV ranges. Dotted lines show areas where the sublevels have the same energy.

large area of uncertainty (see Fig. 2) in the position of the levels.

In Fig. 4 we reproduce the values of g_K and $B_{W.u.}(M1; 3/2^+ \rightarrow 5/2^+)$ with an energy difference between the sublevels of less than 10 eV. The existence of the optical range for the transitions $|5/2^+, F=3\rangle \rightarrow |3/2^+, F=2\rangle'$ and $|3/2^+, F=2\rangle' \rightarrow |3/2^+, F=1\rangle$ is an unusual feature of the MHF structure in $(\mu_{1S_{1/2}}^{-} {}^{229}\text{Th})^*$. It gives hope that advanced optical methods can be applied to the study of this extraordinary nuclear state.

Transitions between sublevels. Both sublevels of the isomeric state $3/2^+$ (7.8 eV) lie below the ground-state sublevel $|5/2^+, F=3\rangle$. As a result, spontaneous transitions to the isomeric level accompanied by its population become possible.

Mixing of sublevels with $F=2$ significantly increases the probability of transitions 2 and 4 in Fig. 2 between the sublevels of the ground and isomeric states. The wave functions of the new sublevels have the form

$$|3/2^+, F=2\rangle' = \sqrt{1-b^2}|3/2^+, F=2\rangle + b|5/2^+, F=2\rangle,$$

$$|5/2^+, F=2\rangle' = -b|3/2^+, F=2\rangle + \sqrt{1-b^2}|5/2^+, F=2\rangle,$$

where $b = (E_{1'} - E_1) / \sqrt{(E_{1'} - E_1)^2 + \mathcal{E}^2} \simeq 0.47$ [43]. Accordingly, the component of the transition, which connects the state $|5/2^+, F=3\rangle$ with $b|5/2^+, F=2\rangle$ makes the main contribution to the transition 2 in Fig. 2. This transition occurs via a spin flip of the muon without changing the nuclear state.

The main decay channel of the $|5/2^+, F=3\rangle$ sublevel is the transition to the $|5/2^+, F=2\rangle$ ground-state sublevel (labeled 1 in Fig. 2). The probability of transition 1 calculated by means of formulas in Refs. [26] and [44] is 2.8×10^{-11} eV.

The transition is accompanied by the emission of conversion electrons. The muon in $(\mu_{1S_{1/2}}^{-} {}^{229}\text{Th})^*$ is practically inside the thorium nucleus. The electronic shell perceives the system “muon + thorium nucleus” as an actinium nucleus of charge 89. Therefore, the internal conversion will take place in the electron shell of the Ac atom. For transition 1 the internal conversion coefficient α_{M1} is equal to 6.6×10^5 (it was found using the code described in [8]) with the full width $\Gamma_{\text{tot}} = 1.8 \times 10^{-5}$ eV. This means that the half-life of the sublevel $|5/2^+, F=3\rangle$ is less than 2.5×10^{-11} s. That is, the relaxation of this level is completed prior to muon absorption ($\sim 10^{-7}$ s) or muon decay (2×10^{-6} s).

Taking into account coefficient b^2 , the radiation width of transition 2 is 1.1×10^{-14} eV and the total width equals 7.0×10^{-7} eV ($\alpha_{M1} = 6.0 \times 10^7$). Thus, the probability of isomeric-state excitation at the decay of the ground state is 3%–4%. Modern muon factories generate 10^5 muonic atoms per second. Thus we can expect the formation of the order of $N_{\text{is}} \simeq 3 \times 10^3$ isomeric nuclei per second. From measurements of the corresponding conversion electrons one can hope to identify experimentally the fast transitions 3, 4, and 5. They are comparable in intensity to transitions 1 and 2. Measurement of the parameters of the transitions can give information about g_K and $B(M1; 3/2^+ \rightarrow 5/2^+)$.

The value $N_{\text{is}} \simeq 3 \times 10^3 \text{ s}^{-1}$ is a lower estimate. The muon capture by atom is followed by a cascade of muon transitions in the atomic shell. The process of nonradiative nuclear excitation by means of direct energy transfer from the excited atomic shell to the nucleus via the virtual X photon is possible if the muon transition is close in energy and coincides in type with the nuclear one (see, for example, [24]). This effect was predicted by Wheeler [16]. In the case of resonant excitation of the levels of the $5/2^+[633]$ rotational band the probability of the population of the $3/2^+[631]$ isomeric state is estimated by 1%–2%. (This value corresponds to the probability of isomer population at the α decay of ${}^{233}\text{U}$, which involves mainly the levels of the $5/2^+[633]$ band in ${}^{229}\text{Th}$.) However, a precise account of the isomer population in muonic transitions can be given only experimentally.

Another interesting consequence of the mixing of $F=2$ states is the possible existence of an $E0$ component at transition 5 in Fig. 2. The $E0$ transition is sensitive to differences in the mean-square charge radii $\langle R_p^2 \rangle$ [45]. The probability of the transition depends on the $E0$ transition strength $\rho(E0)^2$, which is proportional to $b^2(1-b^2)(\langle R_p^2 \rangle_{5/2^+} - \langle R_p^2 \rangle_{3/2^+})^2 / R_0^4$. $\rho(E0)^2 = 0$ in the framework of the simplified model for the charge distribution ρ_p used in this work. In reality, the radii $\langle R_p^2 \rangle_{3/2^+}$ and $\langle R_p^2 \rangle_{5/2^+}$ can differ in magnitude and detection of the $E0$ transition would be a step towards a better understanding of the properties of the low-energy doublet in ${}^{229}\text{Th}$.

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