Anomalous Magnetic Hyperfine Structure of the $^{229}$Th Ground-State Doublet in Muonic Atom

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(Dated: February 19, 2018)

The magnetic hyperfine (MHF) splitting of the ground and low-energy $3/2^+ (7.8 \pm 0.5 \text{ eV})$ levels in the $^{229}$Th nucleus in muonic atom ($\mu_1 S_{1/2}$ $^{229}$Th)$^*$ has been calculated considering the distribution of the nuclear magnetization in the framework of collective nuclear model with the wave functions of the Nilsson model for the unpaired neutron. It is shown that (a) the deviation of MHI structure of the isomeric state exceeds 100% from its value for a point-like 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 takes place, (c) the E0 transition which is sensitive to the differences in the mean-square charge radii of the doublet states is possible between the mixed sublevels with $F = 2$, (d) the MHI splitting of the $3/2^+$ isomeric state may be in the optical range for certain values of the intrinsic $g_K$ factor and reduced probability of the nuclear transition between the isomeric and ground states.

PACS numbers: 23.20.Lv, 36.10.Ee, 32.10.Fn

The unique transition between the low-lying isomeric level $3/2^+ (E_{\text{is}} = 7.8 \pm 0.5 \text{ eV})$ (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 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 a hope for a number of scientific breakthroughs that could have a significant impact on technological development and applications. This is a new metrological standard for time $^3$ $^4$ $^5$ and a laser at nuclear transition in the VUV range $^6$. The relative effect of the variation of the fine structure constant $\varepsilon^2$ (we use the system of units $\hbar = c = 1$) and the strong interaction parameter $m_u / \Lambda_{\text{QCD}}$ $^7$ 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 the ability to use thorium isomer as a probe to study the physicochemical properties of solids $^9$, the cooperative spontaneous emission Dicke $^9$ in the system of excited nuclei $^{229}$Th, accelerated $\alpha$-decay of the $^{229}$Th nucleus via the isomeric state $^{11}$. 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 dielectric, the nucleus can absorb and emit the VUV range photons directly, without interaction with the electron shell $^{11}$. As a result, studying of isomeric state by the optical methods becomes possible $^3$, $^{12}$ $^13$.

In this work the $^{229}$Th ground-state doublet is investigated in muonic atom ($\mu_1 S_{1/2}$ $^{229}$Th)$^*$. The muon on the $1S_{1/2}$ atomic orbit creates a very strong magnetic field at the nucleus $^{14}$ $^{15}$. The interaction of this field with the magnetic moments of nuclear states leads to a magnetic hyperfine (MHI) splitting of nuclear levels (see for example $^{16}$ $^2$ $^8$ and references therein). We demonstrate here that the MHI splitting has a number of non-trivial features in the case of ($\mu_1 S_{1/2}$ $^{229}$Th)$^*$: the partial inversion of nuclear sublevels and spontaneous decay of the ground state into the isomeric state $3/2^+$, the anomaly deviation of MHI structure of the isomeric state from its value for a point-like nucleus, an important role of the dynamic effect of finite nuclear size (or the penetration effect) in the states mixing, the possible existence of the electric monopole transition and optical transitions between the MHI sublevels, etc. This situation is very unusual and looks promising in regard to experimental research.

The Fermi contact interaction. Let us consider the system ($\mu_1 S_{1/2}$ $^{229}$Th)$^*$ which consist of the muon bound on the $1S_{1/2}$ shell of 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

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

where $m_e$ and $m_\mu$ are the masses of the electron and muon, respectively, $\mu_B = e/2m_e$ is the Bohr magneton, $\sigma$ 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{align*}
\begin{cases}
x g'(x) - b(E + 1 - V(x)) x f(x) = 0, \\
x f'(x) + 2 f(x) + b(E - 1 - V(x)) x g(x) = 0.
\end{cases}
\end{align*}

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
the sublevels is determined by the formula leads to a splitting of the nuclear levels. The energy of quantum number the muon density is presented in Fig. 22. and isomeric states and determines the sublevels. The resulting energy values are given in Fig. 2.

The MHF splitting found in the model of the Fermi contact interaction is very significant. However, since the muon density decreases quickly to the nuclear edge the obtained values are grossly overestimated.

The distributed magnetic dipole model. The influence of the finite nuclear size on the MHF splitting was first considered by Bohr and Weisskopf [30]. Later the effect of the distribution of nuclear magnetization on MHF structure in muonic atoms was studied by Le Bellac [31]. According to their works, in the case of deformed nucleus the energy of sublevels is given by Eq. (2), where

\[ E_{\text{int}} = \int d^3r j(r) \mathbf{A}(r) \]  

is the energy of interaction of the muon current \( j(r) = -e\psi_\mu^*(r)\alpha\psi_\mu(r) \) (\( \alpha = \gamma^0\gamma, \gamma \) are the Dirac matrices) with the vector potential of the electromagnetic field \( \mathbf{A}(r) \) generated by the magnetic moment of the nucleus. For a system of “rotating deformed core (with the collective rotating angular momentum \( \mathbf{R} \)) + unpaired neutron (with the spin \( S_n \)”), vector-potential is determined by the relation [31, 31]

\[ \mathbf{A}(r) = -\int d^3R [\rho_n(R)g_S\mathbf{S}_n + \rho_c^{m}(R)g_R\mathbf{R}] \times \nabla \frac{1}{|r - R|} \]

where \( \rho_n(R) \) is the distribution of the spin part of the nuclear moment and \( \rho_c^{m}(R) \) is the distribution of the core magnetization, \( g_S \) is the spin \( g \)-factor, and \( g_R \) is the core gyromagnetic ratio. The distributions \( \rho_n(R) \) and \( \rho_c^{m}(R) \) are normalized: \( \int d^3R \rho_n(R) = 1 \), \( \int d^3R \rho_c^{m}(R) = 1 \).

Here we use the standard nuclear wave function

\[ \Psi_{MK} = \sqrt{(2I + 1)/8\pi^2} D_{MK}(\Omega)\varphi_K(R), \]

where \( D_{MK}(\Omega) \) is the Wigner D-function of the Euler angles are denoted, collectively, by \( \Omega \), \( \varphi_K(R) \) is the wave function of external neutron coupled to the core, \( K \) is the component of \( I \) along the symmetry axis of the nucleus, and \( M \) is the component of \( I \) along the direction of magnetic field.

As follows from Eqs. (4), (5), \( E_{\text{int}} \) consists of two parts. The first part is the interaction of the muon with the external unpaired neutron and the second one is the interaction of the muon with the rotating charged nuclear core. These energies are calculated in accordance with formulas from [31]. In our case of the muon interacts with the nucleus in the head levels of rotational bands (for such states we have \( K = I \)), and two contributions take the following form:

\[ E_{\text{int}}^{\text{core}} = E_0 \frac{I}{I+1} \left( \frac{1}{g_R} \right) \left\{ (\mathcal{M}) - \int \left( \frac{\rho_n(y)}{\rho_c^{m}(R)} \right) d^3y \times \int_y^\infty \left[ 1 - x^2 \left( \frac{\Theta(I, \theta)}{1} \right) \right] f(x)g(x)dx \right\}. \]

Here, \( E_0 = -2e^2M_p/[3(M_pR_0)^2] \), \( g_K \) is the intrinsic \( g \) factor, \( \rho_n(y) = \varphi_K(y)^*\varphi_K(y) \), \( y = \mathbf{R}/R_0 \), \( \Theta(I, \theta) = \sqrt{4\pi/\sqrt{5}}y_{20}(\theta)(2I + 1)/[I(2I + 3)] \). The first term in the
of the states with the 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 the MHF splitting is absent or very weak. Conversely, the magnetic moment of the isomeric level equals to zero for $g_K \approx -0.206$, while the MHF splitting is relatively large. The reason is the following. The magnetic field generated by the spin of the nucleon is sensitive to the non-sphericity of the wave functions $\varphi_K$. This leads to the appearance of the additional factor $\Theta(I, \theta)$ in the spin part of the Eq. (36) [30, 31]. Averaging over the angles reduces the spin contribution in respect to the orbital part. A small imbalance emerged in the system leads to the violation of the “fine tuning” between the spin and 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 the sublevels with $F = 2$.** To find the final position of the sublevels we now consider the mixing of the 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 the energy $E_1$ and the $|5/2^+, F = 2 \rangle$ sublevel with the energy $E_2$ can be found from equations given in Refs. [30, 40]. They generalize the static Bohr-Weisskopf effect for the case of nuclear excitation at the electron (muon) transitions in the atomic shell. For $M1$ transition we obtain

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

where $B_{Wu}(M1; 3/2^+ \rightarrow 5/2^+) = 3.0 \times 10^{-2}$ is the reduced probability of the nuclear isomeric transition in Weisskopf’s units [41]. $\xi$ 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 $\mathcal{E} \simeq 150$ eV.
we reproduce 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. The dotted lines show the areas where the sublevels have the same energy.

Accordingly, the component of the transition, which connects the state $|5/2^+, F = 3\rangle$ with $|5/2^+, F = 2\rangle$ gives the main contribution to the transition 2 in Fig. 2. This transition occurs via a spin flip of the muon without changing nuclear state.

The main decay channels of the $|5/2^+, F = 3\rangle$ sublevel is the transition to the $|5/2^+, F = 2\rangle$ ground state sublevel (labeled as 1 in Fig. 2). The probability of the transition 1 calculated by means of formulas of Refs. 26, 44 is $2.8 \times 10^{-11}$ eV. The transition is accompanied by the emission of conversion electrons. Muon in $(\mu^1S_{1/2}^{229}\text{Th})^+$ is practically inside the thorium nucleus.

Electronic shell perceives the system “muon + Thorium nucleus” as the Actinium nucleus of charge 89. Therefore, the internal conversion will take place in the electron shell of the Ac atom. For the transition 1 the internal conversion coefficient $\alpha_{M1}$ is equal to $6.6 \times 10^5$ (it have been 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 $2.5 \times 10^{-11}$ s. I.e. the relaxation of this level is completed prior to the muon absorption ($\sim 10^{-7}$ s) or the muon decay ($2 \times 10^{-6}$ s).

Taking into account the coefficient $b^2$, the radiation width of the transition 2 is $1.1 \times 10^{-14}$ eV and the total width equals to $7.0 \times 10^{-7}$ eV ($\alpha_{M1} = 6.0 \times 10^5$). Thus, the probability of the isomeric state excitation at the decay of the ground state is 3.4%. Modern muon factories generate of $10^5$ muonic atoms per second. Thus we can expect the formation of the order of $N_{is} \simeq 3 \times 10^3$ isomeric nuclei per second. From the measurements of the corresponding conversion electrons one can hope to identify experimentally the fast transitions 3, 4, and 5. They are comparable in intensity with the transitions 1 and 2. The measurement of the parameters of the transitions can give information about $g_K$ and $B_{W,u} (M1; 3/2^+ \rightarrow 5/2^+)$. The value $N_{is} \simeq 3 \times 10^3 \text{ s}^{-1}$ 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 [10]. 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 the isomer population at the $\alpha$ 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 $F = 2$ states mixing is the possible existence of the $E0$ component at the transition 5 in Fig. 2. The $E0$ transition is sensitive to the differences in the mean-square charge radii $\langle R_p^2 \rangle$ [15]. The probability of the transition depends on the $E0$ transition strengths $\rho(E0)^2$, which is proportional to $b^2(1-b^2)((R_p^2)_{5/2^+}-(R_p^2)_{1/2^+})^2/R_0^4$, $\rho(E0)^2 = 0$ in the framework of the simplified model for the charge distribution $\rho_p$ used in this work. In reality the radii $\langle R_p^2 \rangle_{5/2^+}$ and $\langle R_p^2 \rangle_{1/2^+}$ can differ in magnitude and the detection of the $E0$ transition would be a step towards a better understanding of the properties of the low-energy doublet in $^{229}\text{Th}$.

This research was carried out by a grant of Russian Science Foundation (project No 16-12-00001).

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