PREDICTIONS FOR NUCLEAR SPIN MIXING IN MAGNETIC FIELDS*

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Dedicated to Janusz Dąbrowski in honour of his 65th birthday

Mixing of nuclear states with different spins in external magnetic fields is briefly discussed. A case of special interest is the ^{229}Th nucleus because of its 4.5(1) eV $3/2^+$ excited state which may mix with the $5/2^+$ ground state. Magnetic hfs and mixing of these states are calculated in cases of single electron and muonic atoms. Chances of experimental detection are considered.

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1. Introduction

Energy levels of some systems may split in external magnetic fields. This phenomenon is known and widely used in many fields of physics. The related mixing of states, although known, is studied in some atomic systems

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[1]. An analogous mixing of nuclear states is much more difficult to detect and analyze. To observe it in a nuclear system two conditions should be met:

1. Two basic states of the same parity and spins different by one unit must be sizably mixed.
2. If the system is to be observed by a decay, this decay should be hindered in one of the basic states.

The first condition can be fulfilled only in very strong fields. There are two accessible sources that may generate such fields. One is an atomic electron, preferably an unpaired one in the $1s$ state. Such a situation may be generated in a highly ionized hydrogen-like atom kept within a Paul trap. Heavy hydrogen-like ions are available for experiments at GSI Darmstadt. Another source of magnetic field may be a muon or any other negatively charged particle bound into an exotic atom. The magnetic field of one $1s$ orbital electron may be as strong as 10 MT in heavy nuclei. Still, it is not strong enough to mix nuclear states unless the levels are exceptionally close. The muonic atom offers fields larger by $(m_\mu/m_e)^2$ at a disadvantage of its limited lifetime, however. Also the analysis of the magnetic interactions of muons is complicated by uncertainties related to the nuclear charge distribution. The magnetic interaction energy of the nucleus and electron (muon) may be presented as an operator

$$H_{\rm mag} = -\vec{\mu}\vec{\sigma}_e B_{\rm eff} \,, \tag{1}$$

where $\vec{\mu}$ is a magnetic moment operator of the nucleus, $\vec{j} = \vec{\sigma}_e/2$ is the spin of the electron, and $B_{\rm eff}$ may be interpreted as an analog of the classical external magnetic field. As the average direction of the magnetic moment follows the nuclear spin $\vec{I}$, Eq. (1) has the $\vec{I}\vec{j}$ structure. The energy levels of the system are split into multiplets with the energy shifts given by the Fermi-Segré formula

$$W_{\rm hfs} = A\,C(F, I, j)\,, \tag{2}$$

with

$$C(F, I, j) = \frac{F(F+1) - I(I+1) - j(j+1)}{2Ij}\,. \tag{3}$$

Here, F is the total spin of the system and the magnetic hyperfine constants A are determined by experimental level splittings. In the case of electrons, A yield basically the nuclear magnetic moments μ_I. In the muonic experiments, A depends also on the magnetization distribution in the nucleus, and the μ_I moments if known become additional constraints on the theories used to calculate the hf constants.

Measurements of the fine and hyperfine structure in muonic atoms have become a standard method to determine nuclear electromagnetic properties: charge radii, quadrupole and magnetic moments of nuclei [2]. Also, the mixing of ground and rotational states by quadrupole interactions is well studied in hadronic atoms. An analogous mixing of nuclear states due to magnetic dipole interactions M1 has also been observed [3]. This experiment compares intensities of nuclear M1 transitions in muonic and ordinary atoms of ^{205}Tl and ^{209}Bi. The mixing coefficient of about 1% has been established. This result could have been achieved because of a strong hindrance of the basic M1 transitions. The measurement of the level shifts yields information on magnetic moments and charge radii in the excited states. The level shifts due to magnetic mixing are too minute to be measured for typical 100 keV separations of the nuclear states.

In the case of ordinary atoms, an observation of the magnetic mixing has been considered [4] in connection with an early suggestion of Lyuboshitz *et al.* [5]. It follows from these papers that in most cases the mixing effects are very small. However, it turns out that there exists a unique nucleus of ^{229}Th, where the $3/2^+$ state excited by only 4.5 eV [6] may mix with the ground $5/2^+$ state [7].

It is the aim of this note to calculate the hf structure of these states in the one electron ^{229}Th^{89+}ions and in muonic atoms. The results are given in Section 2. The possibility of the detection of the state mixing is also discussed there. Calculations of the strength of the magnetic field produced by a 1s electron or, an equivalent, B_{eff} due to magnetization of the nucleus are presented in Appendix A.

2. Hyperfine structure in the ^{229}Th

2.1. The level doublet in ^{229}Th

The studies of the ^{233}U $\rightarrow$ ^{229}Th α-decay [6] and the reaction ^{230}Th(d,t)^{229}Th [8] indicate the existence of two $\Delta I = 1$, positive-parity levels in ^{229}Th. These levels, found to be exceptionally close in energy are interpreted as neutron states. Their Nilsson model quantum numbers are given in Table I together with the recent [6] value of the excitation energy and with the magnetic moments used in our calculations of the hyperfine splitting. The moment for the $5/2^+$ ground state is taken from Bemis [9]. Model calculations [10, 11] yield 0.46 μ_N in excellent agreement with this experiment. For the excited $3/2^+$ state, the data available are $g_K = 0.309 \pm 0.016$ [9] and $|g_K - g_R| = 0.60 \pm 0.08$ [12]. The nuclear magnetic moments are generated by two currents: one is due to collective rotation of the deformed nucleus and another comes from the magnetic moment of the valence neutron. The g_R is the g factor in the collective motion while g_K is the g factor related to the neutron moment. The numbers given above lead to two possible values of the magnetic moment, 1.00 or -0.08 μ_N. The latter is chosen as it is close to the theoretical result of -0.05 μ_N [10, 11] and because it is negative, similarly as the magnetic moment of the $3/2^+$ [631] ground state of ^{227}Ra. The reduced M1 transition probability given in Table I has been deduced from the value of $B(\mathrm{M1}, I = 9/2, K = 5/2 \rightarrow I = 7/2, K = 3/2) = 0.032 \pm 0.006\ \mu_N^2$ [9], obtained for another transition between rotational states built on the two levels of interest. The pure-rotation formula was used for this aim, and the value obtained is slightly higher than a theoretical result of 0.039 μ_N^2 [10, 13].

TABLE I

The doublet of nuclear levels in ^{229}Th

Nilsson quantum numbers	Excitation ΔE (eV)	Magnetic moment (μ_N)	$B(M1, 3/2^+ \rightarrow 5/2^+)$ $[\mu_N^2]$
$5/2^+[633]$	0	0.45 ± 0.06	0.069 ± 0.013
$3/2^+[631]$	4.5 ± 1.0	-0.08 ± 0.08	

Nuclear magneton $\mu_N = 3.15\ 10^{-8}$ eV/T. For the energy spacing see [6], for other data see text.

The half-life of the ^{229}Th ground state is known to be 7340 y. It is determined entirely by the probability of the alpha decay. For the $3/2^+$ excited state, the role of the alpha decay is expected to be negligible (see section 2.4). With B(M1) value given in Table I, and level energies assumed to be 3.5, 4.5 and 5.5 eV, a partial half-life for the gamma transition to the $5/2^+$ ground state is 4, 1.7 and 0.9 h, respectively. This is our estimate for the limits of the half-life of the $3/2^+$ state in case of a hydrogen-like ion. On the other hand, in a neutral ^{229}Th atom the half-life of this state could be much shorter because the $3/2^+ \rightarrow 5/2^+$ transition can be highly enhanced due to the role of atomic electrons (the effect of an electron bridge [18]).

2.2. Hyperfine splitting of the levels in $^{229}Th^{89+}$ and ^{229}Th+muon

Now we want to calculate the magnetic field produced at the nucleus by a 1s electron in a hydrogen-like ion. A nonrelativistic formula [14] which assumes a point charge and a point magnetic moment of the nucleus reads:

$$B(0) = \frac{e}{3m_e}|\Psi(0)|^2 = 1.67\ 10^{-5} * Z^3\ [MT], \tag{4}$$

where Ψ is the atomic wave function at the origin. For high Z nuclides Eq. (4) is a poor approximation, and the charge and magnetization distributions as well as relativistic effects must be taken into account. These effects lead to an effective value $B_{\text{eff}} = B(0)F_R$ with an enhancement factor F_R. This procedure is described in more detail in Appendix A and results are given in Table II. In contrast to the electron case the B_{eff} for a muon is lower than the relevant $B(0)$. This happens because muon stays for most of its time within the nucleus.

TABLE II

Magnetic field in MT at the nucleus ^{229}Th

Produced by	1s electron	1s muon
$B(0)$	12	5.2 10^5
B	27.7	2.7 10^5

The interaction between this magnetic field and the nuclear magnetic moment is given by the Hamiltonian of Eq. (1), $H_{\text{mag}} = -\vec{\mu}_I \vec{\sigma}_e B_{\text{eff}}$. The relevant hyperfine-energy shift is $W_{\text{hfs}} = AC$ where now $A = \mu_I B_{\text{eff}}$ and C is given by Eq. (3). In our case $I = 5/2$ or $3/2$, $j = 1/2$ and $F = I \pm 1/2$. The hf splitting energies are shown in Table III. The energy shift due to the nuclear spin mixing has been neglected so far.

2.3. Mixing of the levels in $^{229}Th^{89+}$ and ^{229}Th+muon

Under the assumption of a vanishing nondiagonal matrix element, the two $F = 2$ substates of the nucleus-plus-electron system have well defined nuclear spin. They are spaced by $\Delta E + \Delta W_{\text{hfs}}$. However, the diagonal matrix element which may be expressed as $\langle 3/2|\vec{\mu}\vec{B}_{\text{eff}}|5/2\rangle$ is different from zero. It is related to the reduced M1 transition probability:

$$|\langle 3/2,\ F = 2|H_{\text{mag}}|5/2,\ F = 2\rangle| = \sqrt{\frac{32\pi}{15} B(M1,\ 3/2^+ \to 5/2^+)} B_{\text{eff}}\,. \quad (5)$$

This term mixes the two $F = 2$ components into new states

$$|F = 2,\ \text{lower}\rangle = \sqrt{1 - b^2}|F = 2,\ 5/2^+\rangle + b|F = 2,\ 3/2^+\rangle\,, \quad (6)$$

where b is the mixing amplitude, and an orthogonal upper state. This means that the nuclear ground state wave function acquires an admixture of the $I = 3/2$ component, while the upper state receives an admixture of the $I = 5/2$ component. The distance between the two $F = 2$ substates increases to $\Delta E + \Delta W_{\rm hfs} + \Delta E_{\rm mix}$. The hf separations of $\Delta W_{\rm hfs} = 0.48$ eV (electrons) and 4.68 KeV (muons) follow from Table III. Now the B(M1) value given in Table I is equivalent to the coupling strength of 0.59±0.05 eV (electrons) or 5.8±0.5 keV (muons). The results for the mixing and the separation estimates are given in Table IV for the experimental 3/2 state excitation energy (in the neutral ^{229}Th atom), for the excitation energies different by the experimental error and for a zero spacing.

TABLE III

Hyperfine splitting of the levels in $^{229}Th^{89+}$ and ^{229}Th+1s muon

Quantum I	F	Energy shift $^{229}Th^{89+}$ $W_{\rm hfs}$ (eV)	^{229}Th+1s muon $W_{\rm hfs}$ (keV)
3/2	1	0.12	1.14
3/2	2	−0.07	−0.68
5/2	2	−0.55	−5.36
5/2	3	0.39	3.83

TABLE IV

The nuclear spin mixing in $^{229}Th^{89+}$

ΔE	(eV)	5.50	4.50	3.50	(0)
b^2	(%)	0.95	1.35	2.06	(31)
$\Delta E_{\rm mix}$	(eV)	0.12	0.14	0.17	(0.79)

In the 1s muonic atom the upper state admixture is almost independent on the uncertainty in the excitation energy, $b^2 = 31\%$. Let us notice that the magnetic mixing in this case induces a large level shift, $\Delta E_{\rm mix} = 7.8$ keV. Effects of this magnitude are well within the experimental energy resolution in the muonic X ray measurements.

2.4. The α-decay of ^{229}Th and $^{229}Th^{89+}$

When searching for a process sensitive to the degree of mixing of the $5/2^+$ and $3/2^+$ nuclear levels in ^{229}Th, one should consider, in particular, a comparison of the α decay of the neutral ^{229}Th atom and of the relevant hydrogen-like ion.

In the ^{229}Th$\rightarrow$^{225}Ra+α decay, see Table V, the most intense transition leads to the 236 keV $5/2^+$ level of the daughter nucleus. As manifested by the hindrance factor, it is clearly a favoured transition, which is due to the fact that in the initial and final states the odd neutron occupies the same Nilsson-model orbit. This odd neutron plays the role of the spectator, while the *alpha* particle is emitted by the even-even core.

Table V accounts also for the 150 keV $3/2^+$ level of ^{225}Ra. This level is a Nilsson-orbit analog of the 4.5 eV $3/2^+$ level in ^{229}Th. The alpha transition from the latter level to the 150 keV ^{225}Ra level would be favoured (although it could hardly compete with the gamma transition to the $5/2^+$ ground state of ^{229}Th, see section 2.1.). On the other hand, as a result of the change of the odd-neutron Nilsson orbit, the observed alpha transition between the ^{229}Th ground state and the 150 keV ^{225}Ra level is highly hindered.

TABLE V

Selected data [15] on the α-decay of ^{229}Th to levels in ^{225}Ra

Level in ^{225}Ra		α-transition	
E (keV)	Nilsson state*	branching (%)	hindrance factor
150	$3/2^+$ [631]	0.21	1.4 10^3
236	$5/2^+$ [633]	53	1.57

* Main component.

In ^{229}Th^{89+} the $5/2^+$ nuclear ground state gets an admixture of the $3/2^+$ state of roughly 1%, see Table IV. This admixture would bring a minor reduction of probability for the transition to the 236 keV level. However, at the same time, it would open an additional, unhindered, channel for the decay to the 150 keV level. The $l = 0$ barrier penetrability for the latter transition is about 3.6 times higher than that for the transition to the 236 keV level. One may expect, therefore, that the level mixing would result in the increase of the branching ratio to the 150 keV level from 0.21% (Table V) to few percent. An observation of this change would be an indication of the spin mixing effect.

3. Summary and conclusions

Due to the unusually small energy separation between the $5/2^+$ ground state and the $3/2^+$ excited state in ^{229}Th, this nucleus may be a candidate for the observation of the nuclear-spin mixing in a magnetic field. The field of a sufficiently high strength can be produced at this nucleus by the 1*s* electron in the $^{229}Th^{89+}$ ion. Even much stronger field (by four orders of magnitude) is expected to act on the nucleus in a $^{229}Th+1s$ muon system.

For prediction of the degree of nuclear-spin mixing in $^{229}Th^{89+}$, a quantitative analysis of the magnetic field produced by the $1s$ electron has been performed. The result obtained, $B_{\text{eff}} = 27.7$ MT, is lower by only a few percent than the value derived from the formulae known to apply to the ns electrons ($n \gg 1$) of alkali atoms. One of our conclusions is, therefore, that the latter approach, with tabelarized results available, is good enough for a quick estimate of the spin-mixing effect in nuclei.

The degree of mixing depends very strongly on the energy separation between the states of concern. For the 4.5±1.0 eV energy difference established recently at Idaho Falls for the $3/2^+$ and $5/2^+$ nuclear levels in a natural ^{229}Th atom, the use of the effective magnetic-field value given above leads to the 1–2% mixing in a hydrogen-like ion. We have shown that this mixing could be detected *via* a comparison of the relative intensities of α lines from the decay of ^{229}Th and $^{229}Th^{89+}$. Beams of hydrogen like ions of heavy elements are already available at GSI Darmstadt. However, the experiment with $^{229}Th^{89+}$ would be highly hindered by its very long half-life.

For a ^{229}Th muonic atom, the mixing of the $3/2^+$ and $5/2^+$ levels is predicted to be as high as 31%, but making a ^{229}Th target seems rather unrealistic.

APPENDIX A

Strength of the magnetic interactions

For high Z, relativistic calculations of the atomic magnetic field are required. These are done in this section in two steps: first a vector potential due to the nuclear magnetization is found, then the magnetic interaction is averaged over the atomic $1s$ 1/2 state. In this way one finds the B_{eff} of Eq. (3). This procedure is well known in the studies of hfs and the results may be found in textbooks, *e.g.* that of Kopfermann (1958). There are differences, however, ours is a hydrogen-like system while Kopfermann considers a natural atom with a valence ns electron. One purpose of this section is to compare some approximate expressions for the magnetic field in those two situations.

The situation met in thorium is rather simple. There are two nuclear sources of magnetic field. One is the magnetic moment of the valence unpaired neutron, another is an electric current generated by a collective rotation of the whole nucleus. At first let us discuss the magnetic current due to the neutron rotating around a deformed nuclear core. The intrinsic nuclear spin is oriented along the nuclear symmetry axis while the neutron spin $\vec{s}_n$ is either parallel or anti-parallel to it. The magnetization, due to the neutron anomalous moment ($\vec{\mu}_n = -3.82\mu_N \vec{S}_n$) is $\vec{M}(r) = \vec{\mu}_n \hat{\rho}(r)$, where $\hat{\rho}$ is the neutron density or transition density operator. Now the current is $\vec{j}(r) = -\vec{\partial} \times \vec{M}(r)$ and it generates the vector potential

$$\vec{A}(r) = \tfrac{1}{4\pi} \int \tfrac{dr \vec{j}(r')}{|r-r'|}\,, \tag{A.1}$$

which may be calculated by a multipole expansion of the denominator. The dominant monopole term yields the dipole magnetic term which relates the magnetic Hamiltonian H_{mag} to the nuclear magnetic moment. The subsequent term is a magnetic octupole due to a nuclear quadrupole deformation. In the thorium case the latter is only one percent correction (later omitted). One obtains in this way

$$\vec{A}(r) = \frac{1}{4\pi r^2} \vec{r} \times \vec{\mu}_n n(r)\,,$$

where

$$n(r) = 4\pi \int_0^r \hat{\rho}(r') r'^2 dr'\,, \qquad n(\infty) = 1\,. \tag{A.2}$$

This vector potential enters into the relativistic electron Hamiltonian

$$H_e = \vec{\alpha}(-i\vec{\partial} + e\vec{A}) + \beta m - e\varphi\,. \tag{A.3}$$

An average of the magnetic energy $e\alpha A$ over the unperturbed electron wave function Ψ for the $1s\ 1/2$ state will generate H of Eq. (1). We have:

$$\Psi = \begin{Bmatrix} \frac{G}{r} & U_\alpha \\ \frac{-Fi\vec{\sigma}\vec{r}}{r} & U_\alpha \end{Bmatrix}\,, \tag{A.4}$$

where U_α is a spinor and the radial functions G, F are solutions of the Dirac equations

$$(E - m - e\varphi)G = -F' - \frac{F}{r}\,,$$
$$(E + m - e\varphi)F = G' - \frac{G}{r}\,. \tag{A.5}$$

The electric potential $e\varphi$ is generated by a finite nuclear charge distribution. To indicate explicitly the effect of the latter we write the solutions of Eq. (A.5) in the form

$$G = \Psi(0) \exp\left(\frac{-r}{a_0}\right) \left(\frac{2r}{a_0}\right)^{\gamma-1} \left(\frac{1+\gamma}{\Gamma(1+2\gamma)}\right)^{1/2} * g\,,$$
$$F = -G\frac{1-\gamma}{Z\alpha} * f\,, \tag{A.6}$$

where $a_0 = 1/m\alpha Z$ is the Bohr radius (588 fm) and $\Psi^2(0) = 1/\pi a_0^3$ is the nonrelativistic atomic density at the origin. The $\gamma = \sqrt{1 - Z^2\alpha^2}$ is a parameter which controls relativistic effects, in particular the strength of singularity at the origin. Functions g and f represent corrections due to the finite charge distribution, and for a point charge $f = g = 1$. The magnetic interaction $e\alpha A$ contains $\vec{\alpha} = \begin{pmatrix} 0 & \vec{\sigma} \\ \vec{\sigma} & 0 \end{pmatrix}$, *i.e.*, an operator which mixes large and small components of the Dirac wave function. The matrix element of H between spin states α and β $H_{\alpha\beta} = (U_\alpha, e\vec{\alpha}\vec{A}U_\beta)$ contains angular average over $\hat{r}$ which simplifies the involved spin operator products. The result may be presented as

$$H = -\vec{\mu}_n\vec{\sigma}B(0)F_R \equiv -\vec{\mu}_n\vec{\sigma}B_{\text{eff}}\,, \tag{A.7}$$

with $B(0) = |\psi(0)|^2\frac{e}{3m}$ and

$$F_R = \frac{2}{\Gamma(1+2\gamma)}\int dx e^{-x}x^{2\gamma-2}nfg(x)\,. \tag{A.8}$$

Here, $B(0)$ is the value of magnetic field generated at origin by one non-relativistic electron. Due to finite size effects the field has to be averaged over some region. By relativistic effects it is enhanced to B_{eff} as indicated in Eq. (1) of Section 1. The enhancement factor F_R is usually presented [14] as $F_r(1-\delta)(1-\varepsilon)$ to separate the three effects: enhancement due to the weak singularity of Coulomb wave functions F_r, reduction due to finite charge (δ) and finite magnetization ε. Eq. (A.8) correlates these effects into a double integral. An equivalent, although different in form, result was found by Bohr and Weisskopf [16] and Stroke, Blin-Stoyle, Jaccarino [17] in the usual case of the atomic hfs splitting.

The standard [14] approximate expression $F_R = 3/(4\gamma^2 - 1)$ for a point-like nucleus reflects the singularity of Dirac wave functions at the origin. In this case ($f = 1 = g = n$) the integral (A.8) diverges for $\gamma > 1/2$ or $Z > 118$. Thus the relativistic singularity occurs earlier than for the critical $Z = 1/\alpha = 137$ value. For large Z, however, we find the above approximate formula to be inapplicable. It exceeds the real value (A.8) $F_R = 2\Gamma(2\gamma - 1)/\Gamma(1+2\gamma)$ equal 2.53 at $Z = 90$ by about 20%. The reason for this discrepancy is that the approximate expression is devised for atomic situations of large main quantum numbers n.

Finite size effects constitute a serious correction at high Z. This occurs as a result of a drastic fall off of f and g in the nuclear region. As it was found also on another occasion [16], the charge and magnetization size effects are correlated. Altogether, the reduction amounts to 10.4% and, because of the finite charge distribution effect, the dependence on the details of $n(r)$ is very small. Numerical calculations produce $F_R = 2.29$ and $B_{\text{eff}} = 27.7$

MT. Despite differences in F_r the finite result for F_R is very close to the textbook [14] estimate given in Section 2.

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