

Nuclear anapole moments in single-particle approximation

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Received 3 February 1994; revised 19 April 1994

Abstract

Nuclear anapole moments of ^{133}Cs , $^{203,205}\text{Tl}$, ^{207}Pb , ^{209}Bi are treated in the single-particle approximation. Analytical results are obtained for the oscillator potential without spin-orbit interaction. Then the anapole moments are calculated numerically in a Woods-Saxon potential which includes spin-orbit interaction. The results obtained demonstrate a remarkable stability of nuclear anapole moment calculations in the single-particle approximation.

1. Introduction

The existence of parity nonconservation (PNC) in atoms is firmly established at present (see, e.g., Ref. [1]). To be precise, only the nuclear-spin-independent PNC effects in heavy atoms have been observed up to now. Just these effects are enhanced as Z^2Q . The last enhancement factor, the so-called weak nuclear charge Q which is numerically close to the neutron number $N = A - Z$, is due to the fact that in the nuclear-spin-independent phenomena all the nucleons act coherently.

As to the atomic PNC effects dependent on nuclear spin, they evidently lack this coherent enhancement and are therefore much smaller. There are strong reasons to expect that these effects are dominated by contact electromagnetic interaction of electrons with nuclear anapole moment (AM) [2,3].

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Table 1
Effective constants κ for heavy nuclei

	Nucleus			
	^{133}Cs	$^{203,205}\text{Tl}$	^{209}Bi	^{207}Pb
analytical result [3]	$0.082g_p$	$0.11g_p$	$0.112g_p$	$-0.08g_n$
its value at $g_p = 4$ [3]	0.33	0.44	0.45	
numerical result [3]	$0.062g_p$	$0.095g_p$	$0.078g_p$	$-0.09g_n$
its value at $g_p = 4$ [3]	0.25	0.38	0.31	
[6]	0.14 (0.28)	–	–	–
[7,8]	0.24	(0.24)	(0.24)	–
this work, analytical, $g_p = 4.5$	0.33	0.42	0.45	$-0.09g_n + 0.005$
this work, numerical, $g_p = 4.5$	0.26	0.40	0.29	$-0.10g_n + 0.004$

Anapole is a new electromagnetic moment arising in a system without centre of inversion [4]. It exists even in such a common object as a chiral molecule in a state with nonvanishing angular momentum [5]. Nuclear anapole moment is induced by PNC nuclear forces.

The electromagnetic PNC interaction of electrons with nuclear AM is conveniently characterized in the units of the Fermi weak interaction constant $^4 G = 1.027 \times 10^{-5} m^{-2}$ by a dimensionless parameter κ . (Its definition is given in the next section.) A closed analytical expression has been obtained for this constant [3] within the nuclear shell model under some extra simplifying assumptions. In particular, for ^{133}Cs this model prediction is (at the numerical value of the effective PNC nuclear constant accepted in the paper quoted)

$$\kappa(^{133}\text{Cs}) = 0.33. \quad (1)$$

More reliable numerical calculations with the Woods–Saxon potential including the spin–orbit interaction result at the same PNC nuclear constant in [3]

$$\kappa(^{133}\text{Cs}) = 0.25. \quad (2)$$

The constant $\kappa(^{133}\text{Cs})$ has been calculated also in Ref. [6]. In that paper only the π -meson-exchange contribution to the P -odd nuclear forces has been included. This contribution constitutes roughly a half of the strength of these forces according to the estimates accepted in Ref. [3] (the second half is due mainly to the P -odd ρ -exchange). No wonder therefore that the number 0.14 obtained in Ref. [6] for $\kappa(^{133}\text{Cs})$ constitutes roughly a half of the total result (2). (In Table 1, containing the summary of theoretical results, in the corresponding entry we indicate in brackets what to our guess would be the result of Ref. [6] if the ρ -exchange were included.)

Later numerical calculations with the oscillator potential [7] led at the same value of the P -odd nuclear constant g_p to

$$\kappa(^{133}\text{Cs}) = 0.24. \quad (3)$$

⁴ The system of units with $\hbar = 1$, $c = 1$ is used; m is the proton mass.

Less satisfactory is the agreement between the results for the AM of ^{209}Bi obtained in Refs. [3,7]. As to the AM of $^{203,205}\text{Tl}$ the disagreement between the predictions made in Refs. [3,8] is even stronger. (The values of $\kappa(^{203,205}\text{Tl})$, $\kappa(^{209}\text{Bi})$ at the same magnitude of g_p as accepted in Ref. [3] is not explicitly given in Refs. [7,8]. So, in the corresponding entries of Table 1 we present in brackets our extrapolation of $\kappa(^{203,205}\text{Tl})$, $\kappa(^{209}\text{Bi})$, obtained in Refs. [7,8], from their values of g_p to that accepted in Ref. [3].)

Experiments aimed at the detection of nuclear AM in cesium, thallium, lead, bismuth are underway in many groups. The first evidence of a nuclear-spin-dependent P -odd effect has been seen already in cesium [9]. The result of this experiment is

$$\kappa(^{133}\text{Cs}) = 0.72(39). \quad (4)$$

Therefore, detailed theoretical investigation of various contributions to nuclear AM looks quite relevant.

The present paper is organized as follows. In the next section we describe the constant-core-density approximation which leads to a closed analytical expression for nuclear AM, and introduce some necessary notions and relations. Then we consider a somewhat more sophisticated model which still allows for an analytical treatment. This model gives some idea about the corrections to the above leading approximation. But the most essential part of the paper is devoted to serious numerical calculations using a realistic description of the core density. The nucleon wave functions and Green's functions are obtained with a Woods–Saxon potential which includes the spin–orbit interaction. The contribution of the current generated by the spin–orbit interaction (omitted in Ref. [3]) is taken into account. As distinct from Refs. [7,8], the spin–orbit interaction itself is treated beyond the perturbation theory.

Though the deviations of the contact and spin–orbit currents from naive potential expressions are included, but in all other respects we restrict throughout the present paper to the single-particle approximation, that of a valence nucleon above a spherically-symmetrical core. The many-body effects are certainly of importance for nuclear anapole moments. We shall consider them in future publications.

2. The leading approximation for nuclear anapole moment

PNC interaction in a system (the atomic nucleus is now of interest to us) mixes opposite parity states of the same total angular momentum and creates in it a spin helical structure [1,4]. In this way such a system with nonvanishing magnetic moment acquires a specific configuration of magnetic field, of the type created by the toroidal winding. This is what is called anapole [4].

The AM vector can be conveniently defined as [1–3]

$$\mathbf{a} = -\pi \int d\mathbf{r} r^2 \mathbf{j}(\mathbf{r}), \quad (5)$$

where $\mathbf{j}(\mathbf{r})$ is the current density operator. The vector-potential produced by the AM is

$$A(\mathbf{r}) = -[\mathbf{a}\Delta - \nabla(\mathbf{a}\nabla)] \frac{1}{4\pi r} \rightarrow \mathbf{a}\delta(\mathbf{r}). \quad (6)$$

We omit in the last expression the term $\nabla(\mathbf{a}\nabla)1/4\pi r$, which can be obviously eliminated by a gauge transformation.

When calculating the AM of a heavy nucleus we restrict ourselves to the shell model and one-particle approximation (both in what we will call the leading approximation and beyond it). We shall assume that the nuclear spin I coincides with the total angular momentum of an odd valence nucleon, while the other nucleons form a core with the zero angular momentum. The effective P -odd potential for an external nucleon can be presented as follows:

$$W = \frac{G}{\sqrt{2}} \frac{g}{2m} \boldsymbol{\sigma} [\mathbf{p}\rho(\mathbf{r}) + \rho(\mathbf{r})\mathbf{p}]. \quad (7)$$

Here $\boldsymbol{\sigma}$ and \mathbf{p} are respectively the spin and momentum operators of the valence nucleon, $\rho(\mathbf{r})$ is the density of nucleons in the core normalized by the condition $\int d\mathbf{r} \rho(\mathbf{r}) = A$ (the atomic number is assumed to be large, $A \gg 1$). The numerical value of the dimensionless constant g_p in the case of an external proton is perhaps close to 4–5 (see below). For an external neutron the corresponding constant g_n is smaller, most probably $g_n \ll 1$.

The leading approximation for the AM of a heavy nucleus corresponds to the assumption that the density $\rho(\mathbf{r})$ is constant throughout the space and coincides with the mean nuclear density ρ_0 . This approximation, first used in Ref. [10], is reasonable if the wave function of the external nucleon is mainly localized in the region of the core. The Schrödinger equation for the external nucleon

$$\left[-\frac{1}{2m} \Delta + U(\mathbf{r}) + W(\mathbf{r}) \right] \psi(\mathbf{r}) = E\psi(\mathbf{r}) \quad (8)$$

to first order in W for $\rho(\mathbf{r}) = \rho_0 = \text{const.}$ has the elementary solution

$$\psi(\mathbf{r}) = \left(1 - i \frac{G}{\sqrt{2}} g\rho_0 \boldsymbol{\sigma}\mathbf{r} \right) \psi_0(\mathbf{r}). \quad (9)$$

Here $\psi_0(\mathbf{r})$ is the unperturbed wave function of the external nucleon. It might seem that now interaction (7), which is equivalent to the electromagnetic interaction with a constant vector-potential $\mathbf{A} = -(G/\sqrt{2})(g/e)\rho_0\boldsymbol{\sigma}$, should not result in any physical effects at all. However, the spin part of the current density

$$\mathbf{j}^s(\mathbf{r}) = \frac{e\boldsymbol{\mu}}{2m} \nabla \times (\psi^\dagger \boldsymbol{\sigma}\psi), \quad (10)$$

($\boldsymbol{\mu}$ is the nucleon magnetic moment) does work due to the noncommutativity of the $\boldsymbol{\sigma}$ -matrices, even in this approximation. Simple calculations using formulas (5), (9) and (10) yield

$$a = \frac{Gg\rho_0}{\sqrt{2}} \frac{2\pi e\boldsymbol{\mu}}{m} \langle r^2 \rangle \frac{KI}{I(I+1)},$$

$$K = (I + \frac{1}{2})(-)^{I+1/2-I}. \quad (11)$$

Here l is the orbital angular momentum of the external nucleon. As to its mean square radius $\langle r^2 \rangle$, it coincides to good accuracy with the squared charge radius of the nucleus

$$r_q^2 = \frac{3}{5} R^2 = \frac{3}{5} r_0^2 A^{2/3}, \quad r_0 = 1.2 \text{ fm}. \quad (12)$$

It is useful to present also the effective local AM operator which, acting in the space of nonperturbed wave functions $\psi_0(\mathbf{r})$, produces the result (11). This operator is

$$\hat{a} = \frac{Gg\rho_0}{\sqrt{2}} \frac{2\pi e\mu}{m} [-\sigma r^2 + \mathbf{r}(\sigma\mathbf{r})]. \quad (13)$$

Setting $\rho_0 = (4\pi r_0^3/3)^{-1}$, we finally obtain from (11)

$$a = \frac{G}{\sqrt{2}} \frac{9}{10} g \frac{e\mu}{mr_0} A^{2/3} \frac{KI}{I(I+1)}. \quad (14)$$

The A -dependence of the AM is very natural. Indeed, since the anapole corresponds to the magnetic field configuration induced by a toroidal winding, the AM value should be proportional to the magnetic flux, i.e., to the cross-section area of the torus. This is the origin of $\langle r^2 \rangle$ in formula (11) and of $A^{2/3}$ in (14).

Let us turn now to the PNC problem in atoms. The Hamiltonian of the interaction of an electron with vector-potential (6) can be presented as

$$H_a = e\alpha a \delta(\mathbf{r}) = \frac{G}{\sqrt{2}} \frac{KI\alpha}{I(I+1)} \kappa \delta(\mathbf{r}) \quad (15)$$

($-e$ is the electron charge, α are the Dirac matrices). The Fermi constant G serves as the natural unit for the AM, that arises in first order in the weak interaction, and has the dimension cm^2 . In this unit a convenient characteristic of the nuclear AM for the atomic PNC problem is the dimensionless constant κ . According to (14) it equals [3]

$$\kappa = \frac{9}{10} g \frac{\alpha\mu}{mr_0} A^{2/3}. \quad (16)$$

The enhancement $\sim A^{2/3}$ compensates to a large degree the small fine structure constant $\alpha = 1/137$. That is why the nuclear AM is perhaps the main source of the nuclear-spin-dependent PNC effects in heavy atoms [2,3]. The constants κ for nuclei of experimental interest, as given by simple analytical formula (16), are presented in Table 1. Their numerical values for Cs, Tl, Bi correspond to $g_p = 4$, the number assumed in Ref. [3]. In the next line of Table 1 the results of numerical calculations [3] are presented at the same g_p . Those calculations were performed using a realistic description of the core density $\rho(r)$. The wave function and the Green's function of the valence nucleon were calculated with a Woods-Saxon potential which included the spin-orbit interaction. The crude analytical calculation is obviously in reasonable agreement with that numerical one.

3. Analytical treatment of nuclear AM in a single particle oscillator potential. Contact current contribution

We will start our analysis of various contributions to nuclear AM beyond the leading approximation from a more realistic model which still allows for an analytical treatment. The model consists in the use of the oscillator potential for the valence nucleon and in the neglect of the spin-orbit interaction.

Let us consider first the spin current contribution to the AM. Substituting expression (10) into formula (5) and integrating by parts, we transform the corresponding AM operator to the following form:

$$\hat{a}_s = \frac{\pi e \mu}{m} \mathbf{r} \times \boldsymbol{\sigma}. \quad (17)$$

When using the oscillator potential

$$U(r) = \frac{m\omega^2 r^2}{2} \quad (18)$$

for the valence nucleon, its radius-vector transforms to

$$\mathbf{r} = -\frac{i}{m\omega^2} [H, \mathbf{p}], \quad (19)$$

where H is the valence nucleon Hamiltonian. Substituting this expression into the standard second-order perturbation formula for AM

$$a_s = -i \frac{\pi e \mu}{m^2 \omega^2} \sum_n \frac{\langle 0 | [H, \mathbf{p} \times \boldsymbol{\sigma}] | n \rangle \langle n | W | 0 \rangle + \langle 0 | W | n \rangle \langle n | [H, \mathbf{p} \times \boldsymbol{\sigma}] | 0 \rangle}{E_0 - E_n}, \quad (20)$$

we reduce it by means of the completeness relation to

$$a_s = -i \frac{\pi e \mu}{m^2 \omega^2} \langle 0 | [\mathbf{p} \times \boldsymbol{\sigma}, W] | 0 \rangle. \quad (21)$$

With the explicit form (7) for the weak interaction Hamiltonian W this formula can be rewritten after elementary transformations as

$$a_s = \frac{Gg}{\sqrt{2}} \frac{2\pi e \mu}{m} \frac{KI}{I(I+1)} \frac{1}{m^2 \omega^2} \langle 0 | \rho p^2 - \frac{1}{2} \rho' \partial_r - \frac{l(l+1)}{2Kr} \rho' | 0 \rangle. \quad (22)$$

Let us note here that previously the oscillator-potential model was used in Ref. [11] for the investigation of other P -odd nuclear effects. Then it was applied in Ref. [12] to estimate the contribution of core excitations and to rederive formula (14) (which follows indeed from expression (22) at $\rho(r) = \rho_0 = \text{const.}$ when taking into account the oscillator-potential version of the virial theorem: $\langle 0 | p^2 / m | 0 \rangle = \langle 0 | m\omega^2 r^2 | 0 \rangle$).

We pass over now to the orbital contribution to the AM. As it was demonstrated in Ref. [2], the AM of a charged particle in a spherically symmetrical potential can be presented in the following form:

$$\mathbf{a} = -i \frac{2\pi e}{m} \left(\mu - \frac{1}{3} \right) \frac{KI}{I(I+1)} \sum_n \eta_{0n} r_{0n} - \frac{2}{3} \pi \langle 0 | r^2 \mathbf{j}_c^0 - \mathbf{r} (\mathbf{r} \mathbf{j}_c^0) | 0 \rangle. \quad (23)$$

Here η_{0n} is the P -odd admixture of an intermediate state $|n\rangle$ to the initial one $|0\rangle$ (this coefficient is purely imaginary), r_{0n} is the matrix element of r between those states, j_c^0 is the contact current operator:

$$j_c^0 = ie[W, r] = \frac{Gg}{\sqrt{2}} \frac{e}{m} \rho \sigma. \quad (24)$$

Therefore, to take into account within the simple-minded potential approach the orbital contribution for a proton we should substitute $\mu - \frac{1}{3}$ for μ in formula (22) and add to that expression the following contact term:

$$\frac{Gg}{\sqrt{2}} \frac{2\pi e}{m} \frac{KI}{I(I+1)} \frac{1}{3} \langle 0|r^2\rho|0\rangle. \quad (25)$$

In the case of a valence neutron formula (22) needs obviously no modification within the same model.

However, in fact the contact current contribution both for a valence proton and neutron looks differently. Indeed, let us start from the weak interaction Hamiltonian for the outer nucleon a ($a = p, n$) constructed from corresponding two-body operators (see, e.g., the book in Ref. [1]):

$$W^{(2)} = \frac{G}{\sqrt{2}} \frac{1}{4m} \sum_{a,b} \left\{ (g_{ab}\sigma_a - g_{ba}\sigma_b) \cdot (p_a - p_b), \delta(r_a - r_b) \right\} + g'_{ab} [\sigma_a \times \sigma_b] \cdot \nabla \delta(r_a - r_b), \quad (26)$$

where the notation $\{ , \}$ means anticommutator. After averaging this expression over the core nucleons we obtain formula (7) with

$$g = g_{ap} \frac{Z}{A} + g_{an} \frac{N}{A}. \quad (27)$$

The “best values” [13] of weak coupling constants in the one-meson-exchange approximation lead to the following numbers for the constants discussed [3,14,15]:

$$g_{pp} = g_{nn} = 1.5, \quad g_{pn} = 6.5, \quad g_{np} = -2.2, \quad (28)$$

and correspondingly to

$$g = g_p = 4.5 \quad (29)$$

for the valence proton in Cs, Tl, Bi, and

$$g = g_n \ll 1 \quad (30)$$

for the valence neutron in ^{207}Pb . Here the constants g_{pp} , g_{nn} , g_p and g_n are effective ones, they include already the exchange terms for identical nucleons. These constants include also additional suppression factors reflecting long-range and exchange nature of the P -odd one-meson exchange as well as the short-range nucleon–nucleon repulsion. Their values agree with those obtained in Refs. [16,17] and differ from those given

in Ref. [18] since we include into the ρ -meson exchange the suppression due to the short-range repulsion.

The electromagnetic interaction can be introduced by changing $\mathbf{p} \Rightarrow \mathbf{p} - e\mathbf{A}(\mathbf{r})$. The current density operator is then a derivative of a Hamiltonian over $\mathbf{A}(\mathbf{r})$. This is equivalent to change one power of a momentum operator $\mathbf{p}_a \Rightarrow e_a\delta(\mathbf{r} - \mathbf{r}_a)$ in Hamiltonian. This procedure leads to the following expression for the contact current density operator:

$$\hat{\mathbf{j}}_c = \frac{i}{2} \left\{ \sum_a [W^{(2)}, e_a \mathbf{r}_a], \delta(\mathbf{r} - \mathbf{r}_a) \right\} = \sum_a \mathbf{j}_c^a(\mathbf{r}) \delta(\mathbf{r} - \mathbf{r}_a), \quad (31)$$

where

$$\mathbf{j}_c^a(\mathbf{r}) = \frac{G}{\sqrt{2}} \frac{1}{m} \boldsymbol{\sigma}_a \sum_b (e_a - e_b) g_{ab} \delta(\mathbf{r} - \mathbf{r}_a). \quad (32)$$

For the valence protons $e_a = e$ and this operator reduces to

$$\hat{\mathbf{j}}_c^p = \frac{G}{\sqrt{2}} \frac{e}{m} \boldsymbol{\sigma} g_{pn} \sum_n \delta(\mathbf{r} - \mathbf{r}_n). \quad (33)$$

For the outer neutron ($e_a = 0$) we get

$$\hat{\mathbf{j}}_c^n = -\frac{G}{\sqrt{2}} \frac{e}{m} \boldsymbol{\sigma} g_{np} \sum_p \delta(\mathbf{r} - \mathbf{r}_p). \quad (34)$$

After averaging formulae (33), (34) over the core nucleons we get the following effective contact currents for the valence proton and neutron:

$$\begin{aligned} \mathbf{j}_c^p &= \frac{G}{\sqrt{2}} \frac{e}{m} g_{pn} \frac{N}{A} \rho(\mathbf{r}) \boldsymbol{\sigma} = \mathbf{j}_c^0 + \mathbf{j}_c^1, \\ \mathbf{j}_c^1 &= -\frac{G}{\sqrt{2}} \frac{e}{m} g_{pp} \frac{Z}{A} \rho(\mathbf{r}) \boldsymbol{\sigma}; \end{aligned} \quad (35)$$

$$\mathbf{j}_c^n = -\frac{G}{\sqrt{2}} \frac{e}{m} g_{np} \frac{Z}{A} \rho(\mathbf{r}) \boldsymbol{\sigma}. \quad (36)$$

They differ obviously from the naive ones, \mathbf{j}_c^0 for a valence proton (see (24)) and zero for a valence neutron. Technically it is convenient to retain previous, naive results for anapole moments, supplementing them with the following correction terms:

$$\mathbf{a}^{p1} = -\pi \langle 0 | r^2 \mathbf{j}_c^1 | 0 \rangle, \quad (37)$$

$$\mathbf{a}^{n1} = -\pi \langle 0 | r^2 \mathbf{j}_c^n | 0 \rangle \quad (38)$$

for valence proton and neutron respectively. In this way we get the following closed expression for the AM of a nucleus with a valence proton:

Table 2
Mean squared magnetic radii

Nucleus	$\langle r_m^2 \rangle_{\text{exp}}$	$\frac{3}{5} r_0^2 A^{2/3}$	$\rho^2(N + \frac{3}{2})$
$^{41}\text{Ca}_{20}$	15.92(0.48) [19]	10.27	15.61
$^{45}\text{Sc}_{21}$	12.67(1.57) [20]	10.93	16.11
$^{51}\text{V}_{23}$	12.89(0.72) [20]	11.88	16.79
$^{59}\text{Co}_{27}$	13.99(1.05) [20]	13.09	17.62

$$\begin{aligned}
 a = & \frac{G}{\sqrt{2}} \frac{2\pi e}{m} \frac{KI}{I(I+1)} \langle r^2 \rangle \\
 & \times \langle 0 | g_p \left\{ \mu_p \left[2\rho - \frac{r^2 \rho}{\langle r^2 \rangle} - \frac{1}{2m\omega(N+3/2)} \rho' \left(\partial_r + \frac{l(l+1)}{Kr} \right) \right] \right. \\
 & \left. - \frac{1}{3} \left[2\rho - \frac{2r^2 \rho}{\langle r^2 \rangle} - \frac{1}{2m\omega(N+3/2)} \rho' \left(\partial_r + \frac{l(l+1)}{Kr} \right) \right] \right\} \\
 & - g_p^1 \left(1 - \frac{1}{2K} \right) r^2 \rho | 0 \rangle ; \\
 g_p^1 = g_{pp} \frac{Z}{A} = 0.6, \quad \langle r^2 \rangle = \frac{N+3/2}{m\omega}, \tag{39}
 \end{aligned}$$

where N is the oscillator principal quantum number. In the case of a valence neutron the result is

$$\begin{aligned}
 a = & \frac{G}{\sqrt{2}} \frac{2\pi e}{m} \frac{KI}{I(I+1)} \langle r^2 \rangle \\
 & \times \langle 0 | g_n \mu_n \left[2\rho - \frac{r^2 \rho}{\langle r^2 \rangle} - \frac{1}{2m\omega(N+3/2)} \rho' \left(\partial_r + \frac{l(l+1)}{Kr} \right) \right] \\
 & - g_n^1 \left(1 - \frac{1}{2K} \right) r^2 \rho | 0 \rangle ; \\
 g_n^1 = g_{np} \frac{N}{A} = -1.3. \tag{40}
 \end{aligned}$$

To get the numerical values of nuclear AMs we assume for the core density a step-like profile $f(r)$:

$$\rho(r) = \rho_0 f(r) = \rho_0 \theta(R - r). \tag{41}$$

As to the mean square radius of the valence nucleon $\langle r^2 \rangle$, it is natural to identify it in the shell model with the nuclear magnetic mean square radius $\langle r_m^2 \rangle$. The empirical data on the latter (referring unfortunately to lighter nuclei only) are presented in Table 2. The observation is that in the $^{41}\text{Ca}_{20}$, with a valence neutron, $\langle r_m^2 \rangle$ is close within the error bars to the value predicted by the oscillator model. Meanwhile for nuclei with odd proton, $^{45}\text{Sc}_{21}$, $^{51}\text{V}_{23}$, $^{59}\text{Co}_{27}$, its value is much better approximated by the naive formula (12).

For further calculations it is natural to go over to the usual dimensionless oscillator variable [21]

$$x = \frac{r^2}{\rho^2}, \quad \rho^2 = (m\omega)^{-1} = \frac{4}{5} \left(\frac{2}{3}\right)^{1/3} r_0^2 A^{1/3}. \quad (42)$$

Then the expectation values entering Eqs. (39), (40) reduce to

$$\langle 0|f(r)|0\rangle = \frac{\Gamma(n+l+3/2)}{n!\Gamma^2(l+3/2)} \int_0^x dx e^{-x} x^{l+1/2} F^2(-n, l+3/2, x), \quad (43)$$

$$\langle 0|r^2 f(r)|0\rangle = \rho^2 \frac{\Gamma(n+l+3/2)}{n!\Gamma^2(l+3/2)} \int_0^x dx e^{-x} x^{l+3/2} F^2(-n, l+3/2, x), \quad (44)$$

$$\begin{aligned} & -\frac{1}{2m\omega(N+3/2)} \langle 0|f'(r) \left(\partial_r + \frac{l(l+1)}{Kr} \right) |0\rangle \\ & = 2 \frac{\Gamma(n+l+3/2)}{(N+3/2)n!\Gamma^2(l+3/2)} e^{-X/2} X^{(l+3)/2} \\ & \quad \times F(-n, l+3/2, X) \left(\frac{d}{dX} + \frac{l(l+1)}{2KX} \right) e^{-X/2} X^{l/2} F(-n, l+3/2, X). \end{aligned} \quad (45)$$

Here $X = R^2/\rho^2 = (5/4)(3/2)^{1/3} A^{1/3} = 1.43A^{1/3}$, $F(a, b, x)$ is a degenerate hypergeometric function, $n = (N-1)/2$.

We are interested in the following nuclei:

Cs	$I = 7/2, l = 4, K = 4, N = 4, n = 0, X = 7.304;$
Tl	$I = 1/2, l = 0, K = -1, N = 4, n = 2, X = 8.423;$
Bi	$I = 9/2, l = 5, K = 5, N = 5, n = 0, X = 8.492;$
²⁰⁷ Pb	$I = 1/2, l = 1, K = 1, N = 5, n = 2, X = 8.464.$

For Cs and Bi where $n = 0$ the integrals entering expectation values (43), (44) are nothing else but well-known (and tabulated, see, e.g., Ref. [22]) incomplete gamma-functions, $\Gamma(l+3/2, X)$, $\Gamma(l+5/2, X)$ respectively. In the case of Tl and Pb those expectation values can be also reduced to incomplete gamma-functions.

The numerical results for nuclear AMs, obtained in this model, are presented in Table 1. For Cs, Tl and Bi, at the same value of g_p , they are about 10% smaller than those of the leading approximation. The correction to the spin current contribution constitutes about -4% in Cs and Bi, -7% in Tl. The total contribution of the convection and contact currents is negative in cesium, thallium and bismuth. As to lead, the contact current contribution, though nonvanishing, is very small numerically.

4. Nuclear AM in Woods–Saxon potential. Spin–orbit current contribution

Though being convenient for analytical treatment, the step-like density profile and oscillator model for a single particle potential are however too crude. Moreover, the above analytical model does not take into account the spin–orbit interaction which is, as we will see below, quite essential for numerical results. So, in this section we will describe a numerical treatment of a much more realistic description of a nucleus based on the Woods–Saxon potential including spin–orbit interaction and on a more realistic description of nuclear density.

The profiles of both density and the central part of nuclear potential are known to be similar and well described by a Fermi-type function

$$f(r) = \frac{1}{1 + \exp[(r - R)/a]} . \quad (46)$$

So, the total single-particle potential $U(r)$ has been chosen in a standard Woods–Saxon form

$$U(r) = U_0 f(r) + U_{ls} \frac{1}{r} \frac{df(r)}{dr} (\mathbf{l}\boldsymbol{\sigma}) + U_C(r) , \quad (47)$$

where $U_C(r)$ is the Coulomb potential of a uniformly charged sphere. In order to study the stability of AM calculations against variations of the single particle potentials, we shall use several sets of the Woods–Saxon potential parameters [21,23].

The solution of Eq. (8) can be presented in a form similar to (9),

$$\begin{aligned} \psi(\mathbf{r}) &= \psi_0(\mathbf{r}) + \delta\psi(\mathbf{r}) \\ &= \left(R_0(r) - i \frac{G}{\sqrt{2}} g\rho_0(\boldsymbol{\sigma}\mathbf{n}) \delta R(r) \right) \Omega_{lm}(\mathbf{n}) , \end{aligned} \quad (48)$$

where $\Omega_{lm}(\mathbf{n})$ is a spherical spinor, $\mathbf{n} = \mathbf{r}/r$. The correction $\delta\psi$ is of parity opposite to that of the initial state ψ_0 . The radial function $\delta R(r)$ is normalized in such a way that without spin–orbit potential and for constant density it is (see (9))

$$\delta R(r) = rR_0(r) . \quad (49)$$

This correction can be expressed via the Green's function $G_{ll'}(r, r')$ of the unperturbed radial Schrödinger equation for the orbital angular momentum $l' = 2l - l$:

$$\begin{aligned} \delta R(r) &= -\frac{1}{2m} \int r'^2 dr' \left(\frac{d}{dr'} G_{ll'}(r, r') R_0(r') - G_{ll'}(r, r') \frac{d}{dr'} R_0(r') \right. \\ &\quad \left. - \frac{2K}{r'} G_{ll'}(r, r') R_0(r') \right) f(r') . \end{aligned} \quad (50)$$

After presenting the Green's function through two linearly independent solutions of the radial Schrödinger equation we get

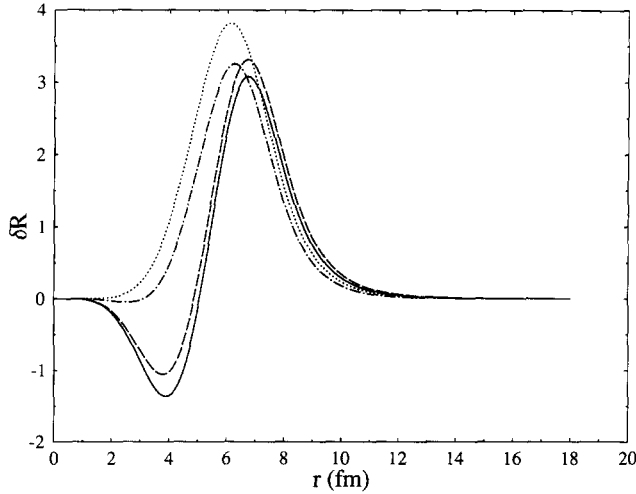


Fig. 1. First order correction $\delta R(r)$ to radial wave function of $1h_{9/2}$ level. Dotted line corresponds to constant density and no spin-orbit potential ($\delta R = rR(r)$). Dash-dotted line refers to varying density and no spin-orbit potential. Dashed line refers to constant density, spin-orbit potential included. Full line corresponds to full potential and varying density.

$$\begin{aligned}
 \delta R(r) = & \frac{u_{II'}^{(1)}(r)}{r} \int_r^\infty dr' \left(u_{II'}^{(2)}(r') u_0'(r') - u_{II'}^{(2)'}(r') u_0(r') \right) \\
 & + \frac{2K}{r'} u_{II'}^{(2)}(r') u_0(r') \Big) f(r') \\
 & + \frac{u_{II'}^{(2)}(r)}{r} \int_0^r dr' \left(u_{II'}^{(1)}(r') u_0'(r') - u_{II'}^{(1)'}(r') u_0(r') \right) \\
 & + \frac{2K}{r'} u_{II'}^{(1)}(r') u_0(r') \Big) f(r'), \quad (51)
 \end{aligned}$$

where $u_0(r) = rR_0(r)$; $u^{(1)}(r)$ and $u^{(2)}(r)$ are solutions regular at the origin and at the infinity respectively. Those last two solutions are normalized to the unit Wronskian: $u^{(1)}u^{(2)'} - u^{(1)'}u^{(2)} = 1$.

The results of this calculation of the δR for $1h_{9/2}$ proton state in ^{209}Bi together with the leading approximation (49) are shown in Fig. 1. In the same picture we demonstrate how δR is influenced by the spin-orbit potential, as well as by the deviation of the density from a constant one. The real form of δR differs considerably from the leading approximation, due mainly to the spin-orbit interaction. As to the realistic density profile, it makes δR slightly smaller as compared to the constant density approximation.

All contributions to the anapole moment can be expressed via the radial correction δR . The spin current term can be obtained from Eq. (11) by substituting

$$(\delta R|r|R_0) = \int_0^\infty r^2 dr \delta R(r)rR_0(r) \quad (52)$$

for $\langle r^2 \rangle$. So, this contribution to the dimensionless anapole constant equals

$$\kappa_s = 2\pi g \frac{\alpha\mu\rho_0}{m} (\delta R|r|R_0). \quad (53)$$

To obtain the convection current contribution we substitute corresponding current density operator

$$\hat{j}_{\text{conv}}(\mathbf{r}) = -i \frac{e}{2m} \sum_p \{ \nabla_p, \delta(\mathbf{r} - \mathbf{r}_p) \} \quad (54)$$

into formula (5) which gives

$$a_{\text{conv}} = -\pi \langle \delta\psi | \left\{ \frac{\mathbf{p}}{m}, r^2 \right\} | \psi_0 \rangle \quad (55)$$

and

$$\kappa_{\text{conv}} = -\pi g \frac{\alpha\rho_0}{mK} (\delta R|r^2 \left(\frac{d}{dr} + \frac{K+2}{r} \right) |R_0). \quad (56)$$

When calculating the contact current contributions it is convenient again to split it into the “naive” part arising from a single particle potential (and vanishing for a valence neutron) and the part which is due to the current densities (35), (36).

The contribution of the total contact current (35) to the AM can be expressed via radial matrix element as

$$\kappa_c = \kappa_c^0 + \kappa_c^1, \quad \kappa_c^i = \pi g^i \frac{\alpha\rho_0}{m} \left(1 - \frac{1}{2K} \right) \langle r^2 f(r) \rangle, \quad i = 0, 1, \quad (57)$$

where $g_p^0 = g_p$, $g_n^0 = 0$, and $g_{p,n}^1$ were defined in (39), (40).

One more term in AM originates from the momentum dependence of spin-orbit interaction. As it will be seen below, this is the most significant correction to the leading approximation. The spin-orbit term in a single particle potential (47) for a proton generates the electromagnetic current density

$$\hat{j}_{ls}^0 = ie[U(r), \mathbf{r}] = eU_{ls} \frac{df(r)}{dr} \boldsymbol{\sigma} \times \mathbf{n}. \quad (58)$$

For an outer neutron the corresponding current density vanishes. The spin-orbit contribution to the proton AM and to κ is respectively:

$$\begin{aligned} a_{ls}^0 &= 2\pi \frac{G}{\sqrt{2}} eg\rho_0 U_{ls} (\delta R|r^2 f'(n(\boldsymbol{\sigma}n) - \boldsymbol{\sigma})|R_0) \\ &= 2\pi \frac{G}{\sqrt{2}} eg\rho_0 U_{ls} (\delta R|r^2 f'|R_0) \frac{KI}{I(I+1)}, \end{aligned} \quad (59)$$

$$\kappa_{ls}^0 = 2\pi\alpha g\rho_0 U_{ls} (\delta R|r^2 f'|R_0). \quad (60)$$

However, as it was the case with the contact current, this is not the complete result. The true spin-orbit current must be obtained from two-particle spin-orbit interaction which can be written as

$$U_{ls}^{(2)} = \frac{1}{2} \sum_{ab} U_{ls}^{ab} (\mathbf{p}_a - \mathbf{p}_b) \cdot (\boldsymbol{\sigma}_a + \boldsymbol{\sigma}_b) \times \nabla \delta(\mathbf{r}_a - \mathbf{r}_b). \quad (61)$$

Averaging it over nuclear core we obtain the spin-orbit part of the single-particle potential (47) with

$$U_{ls} = \left(U_{ls}^{ap} \frac{Z}{A} + U_{ls}^{an} \frac{N}{A} \right) \rho_0. \quad (62)$$

The spin-orbit interaction constants were fitted in Ref. [24]:

$$\begin{aligned} U_{ls}^{pp} &= U_{ls}^{nn} = 36.6 \text{ MeV} \cdot \text{fm}^5, \\ U_{ls}^{pn} &= U_{ls}^{np} = 134.3 \text{ MeV} \cdot \text{fm}^5. \end{aligned} \quad (63)$$

A word of caution is proper here. We will understand expression (61) as a local limit for an operator of a nucleon-nucleon interaction with the proper tensor structure. For identical nucleons the exchange interaction doubles the direct one. The values of U_{ls}^{pp} , U_{ls}^{nn} presented in (63) are just those doubled, effective constants.

The spin-orbit current density from the interaction (61) is

$$\begin{aligned} \hat{\mathbf{j}}_{ls} &= i \sum_a [U_{ls}^{(2)}, e_a \mathbf{r}_a] \delta(\mathbf{r} - \mathbf{r}_a) \\ &= \sum_{ab} U_{ls}^{ab} e_a \delta(\mathbf{r} - \mathbf{r}_a) (\boldsymbol{\sigma}_a + \boldsymbol{\sigma}_b) \times \nabla \delta(\mathbf{r} - \mathbf{r}_b). \end{aligned} \quad (64)$$

This expression for the two-particle spin-orbit current density was used earlier in the description of magnetic properties of a nucleus in Ref. [25]. Including the spin-orbit current into the theoretical description of nuclear magnetic moments and magnetic transition amplitudes improves the agreement with experiment.

In the current density generated by the pp part of operator (61) the exchange and direct contributions cancel each other, i.e., the contact spin-orbit pp interaction does not generate a current at all. Then, averaging expression (64) over the core nucleons and separating the single particle contribution (58), as in the case of the contact current, we get the following effective spin-orbit current for the valence proton:

$$\begin{aligned} \mathbf{j}_{ls}^p &= e U_{ls}^{pn} \rho_0 \frac{N}{A} \frac{df(r)}{dr} \boldsymbol{\sigma} \times \mathbf{n} = \mathbf{j}_{ls}^0 + \mathbf{j}_{ls}^1; \\ \mathbf{j}_{ls}^1 &= -e U_{ls}^{pp} \rho_0 \frac{Z}{A} \frac{df(r)}{dr} \boldsymbol{\sigma} \times \mathbf{n}. \end{aligned} \quad (65)$$

The correction \mathbf{j}_{ls}^1 to the “naive” spin-orbit proton current is relatively small being suppressed by a factor

$$\xi = - \frac{Z U_{ls}^{pp}}{Z U_{ls}^{pp} + N U_{ls}^{pn}}$$

as compared to the potential part. This factor constitutes -0.16 for cesium and -0.15 for thallium and bismuth.

It is noteworthy that even for a valence neutron the spin-orbit current does not vanish. It is generated by the neutron-proton interaction and equals

$$\mathbf{j}_{ls}^n = -eU_{ls}^{np} \frac{Z}{A} \rho(r) \nabla \times (\psi^\dagger(\mathbf{r}) \boldsymbol{\sigma} \psi(\mathbf{r})) . \quad (66)$$

This expression is similar to the spin current density (10) and renormalizes in an obvious way the magnetic moment of an outer neutron.

It is convenient to single out in the sum of all contributions to the effective constant κ

$$\kappa = \kappa_s + \kappa_{ls}^0 + \kappa_{ls}^1 + \kappa_{\text{conv}} + \kappa_c^0 + \kappa_c^1 = \kappa^0 + \kappa_{ls}^1 + \kappa_c^1 , \quad (67)$$

the “naive” potential one κ^0 . The corrections to it κ_{ls}^1 and κ_c^1 in fact go beyond the single-particle approximation. The single-particle contribution can be written in a more compact form, analogous to (23):

$$\mathbf{a}^0 = \left(1 - \frac{1}{3\mu}\right) \mathbf{a}_s + \frac{2}{3} \mathbf{a}_{ls}^0 - \frac{2}{3} \pi \langle 0 | r^2 \mathbf{j}_c^0 - \mathbf{r}(\mathbf{r} \mathbf{j}_c^0) | 0 \rangle . \quad (68)$$

This expression was used to check the accuracy of our numerical calculations which turned out very high.

To study the stability of AM calculations under the variations of the single-particle potential we performed them for two sets of the Woods-Saxon potential parameters (47). In both sets the radii and diffuseness parameters, R and a , are the same for the profiles of central and spin-orbit parts of potential.

The first set is [21]

$$\begin{aligned} R = R_{ls} = 1.27A^{1/3} \text{ fm}, \quad a = a_{ls} = 0.67 \text{ fm}, \\ U_0 = \left(-51 \pm 33 \frac{N-Z}{A}\right) \text{ MeV}, \quad U_{ls} = -0.35U_0, \end{aligned} \quad (69)$$

where the signs $+$ and $-$ refer to neutrons and protons respectively.

The second set [23] has somewhat different parameters, but gives as good fit to the single-particle level positions. It is

$$\begin{aligned} R = R_{ls} = 1.24A^{1/3} \text{ fm}, \quad a = a_{ls} = 0.63 \text{ fm}, \\ U_0 = \left(-53.3 \pm 33.6 \frac{N-Z}{A}\right) \text{ MeV}, \\ U_{ls} = -0.263 \left(1 + 2 \frac{N-Z}{A}\right) U_0. \end{aligned} \quad (70)$$

In both cases we assume the same values of the density parameters [21]:

$$R = 1.11A^{1/3} \text{ fm}; \quad a = 0.54 \text{ fm}, \quad \rho_0 = 0.17 \text{ fm}^{-3}. \quad (71)$$

Table 3

Different contributions to the effective constant κ

Nucleus	^{133}Cs	$^{203,205}\text{Tl}$	^{209}Bi	^{207}Pb
κ_s^a	0.317	0.485	0.376	$-0.099g_n$
κ_s^b	0.301	0.463	0.349	$-0.095g_n$
κ_s^c	0.310	0.497	0.353	$-0.099g_n$
κ_{ls}^0	-0.088	-0.120	-0.126	0
κ_{ls}^1	0.014	0.018	0.019	$-0.006g_n$
$\delta\kappa_{ls}^0$ ^a	0.003	0.019	-0.003	0
$\delta\kappa_{ls}^1$ ^b	0.01	0.032	0.014	0
κ_{conv}^c	-0.019	-0.055	-0.019	0
κ_c^0	0.048	0.064	0.070	0
κ_c^1	-0.007	-0.008	-0.009	0.004
κ^a	0.268	0.396	0.309	$-0.105g_n + 0.004$
κ^b	0.258	0.383	0.298	$-0.101g_n + 0.004$
κ^c	0.257	0.396	0.289	$-0.105g_n + 0.004$

^a The potential parameters from Ref. [21] (see Eq. (69)).

^b The potential parameters from Ref. [23] (see Eq. (70)).

^c The consistent LS-parameters (see Eq. (72)).

The results of calculations obtained for both sets are listed in Table 3. The main contribution to AM, as expected, comes from the spin current. The variation of the parameters of potential changes this term by 3–6%. The next in magnitude term is due to the potential part of spin-orbit current, it constitutes about 30% of the spin current contribution.

In the calculations based on the sets of parameters (69) and (70) the LS-potential was not consistent with the two-particle LS-interaction (61). So, the potential LS-contribution to the AM was calculated in two ways. First, starting from the LS-potential itself. Second, it was obtained from the spin-orbit potential constructed from the two-particle interaction (61)–(63). The difference between second and first ways of calculation is listed as $\delta\kappa_{ls}^0$ in Table 3. It is only natural to perform a consistent calculation, choosing the amplitude of LS-potential in accordance with (62), (63), and its radius and diffuseness parameters the same as those of nuclear density. In this way we come to the third, LS-consistent, version of the potential:

$$R = 1.27A^{1/3} \text{ fm}, \quad a = 0.67 \text{ fm}, \quad U_0 = \left(-51 \pm 33 \frac{N-Z}{A} \right) \text{ MeV},$$

$$R_{ls} = 1.11A^{1/3} \text{ fm}, \quad a_{ls} = 0.54 \text{ fm}, \quad U_{ls} = \left(14.5 \mp 8.3 \frac{N-Z}{A} \right) \text{ MeV}. \quad (72)$$

We kept the central potential parameters as in (69) because it gave smaller $\delta\kappa_{ls}^0$. The calculation based on this version of the potential give $\delta\kappa_{ls}^0 = 0$.

It is noteworthy that the sum of all contributions to AM is less sensitive to a specific potential than each of them taken separately. Its variation does not exceed 5% when going from one set of parameters to another.

We believe that the results obtained with the LS-consistent potential are the most reliable ones. They are presented in the last line of Table 1.

5. Discussion of the results

Let us discuss now why the present results differ from those obtained in Refs. [3,7,8].

As distinct from Ref. [3], we have included now the contribution of the spin-orbit current which turns out quite essential.

On the other hand, the Woods-Saxon potential used here for numerical calculations is more realistic than the oscillator one used for those calculations in Refs. [7,8]. Then, in Refs. [7,8] the spin-orbit interaction is treated perturbatively, while in the present work it is treated exactly. Let us note here again that the oscillator potential without spin-orbit interaction allows one to get an exact analytic solution for the AM, as it has been done in Section 3 of the present work.

To summarize the comparison, we wish to say that the above arguments can serve as serious grounds to consider the numerical results of the present work to be the most reliable ones for the single-particle approximation.

However, accurate quantitative predictions for nuclear AMs cannot be made without proper treatment of nuclear many-body effects. As to the core excitations by the weak interaction Hamiltonian (26), their contribution to nuclear AM has been demonstrated to be small [12]. However, the problem of the configurations mixing caused by usual P -even residual nucleon-nucleon interaction is here much more serious than in the case of nuclear magnetic moments (or the second neutral current constant [7]). The point is that in the last cases it is the specific, kinematical, nature of the operator σ which allows one to restrict with a reasonable accuracy to the excitations within a spin-orbit doublet only. As to the AM, even if the multiconfiguration problem could be reduced to the calculations with the effective operator (13) (which demands a special proof by itself), that operator is coordinate-dependent and in this sense resembles more the magnetic octupole operator than the magnetic dipole one. And many-body effects can renormalize the M3 operator much more strongly than the M1 operator. A drastic example in this respect is ^{209}Bi where the one-particle value of the magnetic octupole moment is almost four times smaller than the experimental one [25].

Let us note here that due to the theoretical uncertainties discussed, in the situation when the AM contribution dominates essentially atomic nuclear-spin-dependent PNC effects, the proposal [7] to single out in those effects the true neutral current contribution by combining experimental data from various heavy nuclei, does not look realistic.

In conclusion it should be emphasized however that even with all those theoretical uncertainties kept in mind, the problem of experimental observation of a new physical phenomenon, nuclear anapole moment, is a fascinating one. Moreover, if the theoretical results of the one-particle approximation, which are by themselves remarkably stable by nuclear standards, will be supplemented by a serious treatment of many-body effects, those experimental investigations will give reliable quantitative information on P -odd nuclear forces.

Acknowledgement

One of the authors (I.B.Kh.) wishes to thank the Institute for Nuclear Theory, University of Washington, and the theoretical physics groups of the Universities of New South Wales, Melbourne and Cambridge, where part of this work was done, for their kind hospitality.

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