Manifestation of the Nuclear Anapole Moment in M1 Transitions in Thallium

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Abstract

Parity non-conservation in atoms is now well established and precision experiments with Cs and Tl allowed to test electroweak theory at low energies. In the Cs experiment the first measurement of the anapole moment (AM) of the nucleus was also made. AM is the P-odd nuclear moment, which appears due to parity non-conserving interactions between the nucleons. Experimental study of AMs of different nuclei can provide unique information about P-odd nuclear forces.

We calculate AM contribution to parity non-conserving $E1$-amplitudes for optical transition $6p_{1/2,F} \to 6p_{3/2,F'}$ and for hyperfine transition $6p_{1/2,F} \to 6p_{1/2,F'}$ in ^{205}Tl. Experimental limit on the former amplitude placed by Vetter *et al.* [PRL,**74**,2658 (1995)] corresponds to the anapole moment constant $\kappa_a = -0.26 \pm 0.27$.

The more direct observation of the AM can be made for the hyperfine transition in the ground state $6p_{1/2}$. The parity non-conservation for this transition is comparable to that for the hyperfine transition in Fr and is an order of magnitude larger than in Cs (it scales roughly as Z^2). Although $M1$ amplitude for the hyperfine transition in Tl is significantly weaker than in Fr, it would be much easier to do the experiment with stable Tl, than with radioactive Fr.

In 1980 Flambaum and Khriplovich [1] pointed out that the nuclear spin-dependent (NSD) part of the parity non-conserving (PNC) interaction in heavy atoms is dominated by the contribution of the anapole moment (AM) of the nucleus [2]. After that AM was observed in the PNC experiment with ^{133}Cs [3], where the measured value of the AM constant κ_a appeared to be even larger than theoretical prediction for the "best values" of the constants of the nuclear PNC interaction (see [4] and references therein). On the other hand, in the most accurate measurement of the PNC amplitudes $6p_{1/2,F} \to 6p_{3/2,F'}$ in ^{205}Tl [5], the NSD amplitude was found to be consistent with zero and smaller than theoretical predictions [4, 6].

In Ref. [6] the ratio between NSD amplitude and the dominant nuclear spin-independent (NSI) PNC amplitude was calculated in the one-particle approximation. Here we recalculate this ratio using CI+MBPT method [7–9], which allows to account for both core-valence and valence-valence correlations. We found that correlation corrections are relatively large, but do not explain the discrepancy between the measurement [5] and the theory [4]. A more accurate measurement of NSD amplitude in the optical transition $6p_{1/2,F} \to 6p_{3/2,F'}$ is hampered by the much larger NSI amplitude and by the smallness of the hyperfine structure of the upper state. Consequently, it may be easier to measure PNC amplitude for the hyperfine transition $6p_{1/2,F} \to 6p_{1/2,F'}$, where NSI amplitude turns to zero, while NSD amplitude is not suppressed [10]. Here we find correlation corrections to this amplitude to be 20%.

In the PNC experiments on the $6p_{1/2} \to 6p_{3/2}$ transition in Tl, the ratio:

$$\mathcal{R} \equiv \mathrm{Im}(E1_{\mathrm{PNC}}/M1) \tag{1}$$

of the PNC amplitude to the magnetic amplitude was measured with 1% accuracy in Ref. [5] and with 3% accuracy in Ref. [11]. In those experiments the hyperfine structure of the lower level $6p_{1/2}$ was resolved. That allowed to determine $\mathcal{R}(F)$ for two hyperfine levels $F = 0$ and $F = 1$ of the ground state. For the level $F = 0$ the only transition to $F' = 1$ of the level $6p_{3/2}$ is allowed, while for the level $F = 1$ transitions to both upper hyperfine levels $F' = 1, 2$ are allowed. Accordingly, $\mathcal{R}(1)$ is some average for two transitions:

$$\mathcal{R}(0) \equiv \mathcal{R}(0,1), \tag{2a}$$
$$\mathcal{R}(1) \equiv x^2\mathcal{R}(1,1) + (1-x^2)\mathcal{R}(1,2), \tag{2b}$$

where coefficient x^2 depends on the intensity of the transitions and on experimental conditions, such as line width and optical depth.

Observation of the F-dependence of the PNC amplitude is important as it can give information about NSD part of the PNC interaction:

$$H_{\rm PNC} = H_{\rm NSI} + H_{\rm NSD} = \frac{G_F}{\sqrt{2}}\Big(-\frac{Q_W}{2}\gamma_5 + \frac{\kappa}{I}\vec{\alpha}\vec{I}\Big)\rho(\vec{r}), \tag{3}$$

where $G_F = 2.2225\times10^{-14}$ a.u. is the Fermi constant of the weak interaction, Q_W is the nuclear weak charge, κ is the dimensionless coupling constant, γ_5 and $\vec{\alpha} \equiv \gamma_0\vec{\gamma}$ are the Dirac matrices, $\vec{I}$ is the nuclear spin ($I = \frac{1}{2}$ for both stable isotopes ^{205}Tl and ^{203}Tl), and $\rho(\vec{r})$ is the nuclear density distribution.

There are three main contributions to the coupling constant κ in NSD part of the PNC interaction (3):

$$\kappa = -\frac{2}{3}\kappa_a + \kappa_2 + \kappa_{Q_W}, \tag{4}$$

where AM contribution is given by the constant κ_a [1], the constant $\kappa_2 = \frac{\lambda}{2}(4\sin^2\theta_W - 1) \approx -0.06$ corresponds to the NSD weak neutral currents [1]. The term κ_{Q_W} is induced by the interference of the NSI interaction with the hyperfine interaction. For heavy nuclei this constant is proportional to $A^{2/3}$ [12, 13], and for Tl $\kappa_{Q_W} \approx 0.02$. Substituting these numbers in (4), we get:

$$\kappa = -\frac{2}{3}\left(\kappa_a - 0.06\right). \tag{5}$$

Theoretical predictions for AM constant depend on nuclear model and vary within the range $0.1 \le \kappa_a \le 0.4$ (see [4] and references therein). On the other hand, for a given nuclear model, one can use measured values of κ_a to get information on the coupling constants of the nuclear P-odd interaction [14–16].

In this article we calculate the NSD amplitudes $6p_{1/2,F} \to 6p_{3/2,F'}$ and use Eq. (5) and experimental results from [5] to place a limit on the AM constant κ_a. Following [5, 6] we use parametrization:

$$\mathcal{R}(F,F') = C(Z)[Q_W - 6\kappa\xi(F,F')], \tag{6}$$

[1] Note, that radiative corrections can change κ_2 quite noticeably.

that links NSD amplitude to NSI one via the function $\xi(F,F')$. According to (2), one can define a function $\xi(F)$ as follows:

$$\xi(0) = \xi(0,1), \tag{7a}$$

$$\xi(1) = x^2\xi(1,1) + (1-x^2)\xi(1,2). \tag{7b}$$

An important property of the one-particle approximation is the equality $\xi(1,1) = \xi(1,2)$ [6], which means that $\xi(1)$ does not depend on the coefficient x^2 in (2b) and (7b). Numerical values, obtained in [6], are:

$$\xi_{\rm op}(0) = 0.87; \qquad \xi_{\rm op}(1) = -0.29\,. \tag{8}$$

In general, when electron correlations are taken into account, $\xi(1,1) \neq \xi(1,2)$. Then, one has to use Eq. (6) for $\mathcal{R}(F,F')$ and calculate function $\xi(F',F)$. After that, experimental function $\xi(F)$ is given by (7). Consequently, the separation of NSI and NSD amplitudes depends on the factor x^2.

NSI amplitude was studied many times, the most advanced and accurate calculations being [17, 18] (for earlier references see [19]). It was shown there that many-body corrections to PNC amplitudes in Tl can be important. That stimulated us to recalculate function $\xi(F,F')$. We follow here the same procedure, which was used in [18]. It is based on the combination of the many-body perturbation theory for core-valence correlations and the configuration interaction for three valence electrons (CI+MBPT method) [7–9].

Most of the technical details of this calculation, such as basis sets, configuration sets, etc., are the same as in Ref. [18], where a number of test calculations were made for the spectrum, hyperfine constants, $E1$-amplitudes, and polarizabilities. All these parameters were shown to be in good agreement with the experiment. That allowed to estimate the accuracy of the calculation of NSI amplitude to be better than 3%. Here we use the same wave functions for the states $6p_j$, but neglect several smaller corrections, such as structural radiation, to the effective operators for valence electrons. The normalization correction is the same for NDI and NSD amplitudes and does not affect the function $\xi(F,F')$.

In order to find PNC amplitude we solve inhomogeneous equations:

$$(E_{6p_{3/2}} - H^{\rm eff})\Psi^{(D)}_{a,m} = D^{\rm eff}_z \Psi_{6p_{1/2},m}, \tag{9}$$

$$(E_{6p_{1/2}} - H^{\rm eff})\Psi^{(D)}_{b,m} = D^{\rm eff}_z \Psi_{6p_{3/2},m}, \tag{10}$$

where $H^{\rm eff}$ is the effective Hamiltonian for valence electrons, which accounts for core-valence correlations within the second order many-body perturbation theory [7, 8], $D_z^{\rm eff}$ is z-component of the effective $E1$-amplitude in the length-gauge [20], and m is magnetic quantum number. Solutions of these equations can be decomposed in terms with definite angular quantum number J:

$$\Psi_{i,m}^{(D)} = \sum_J \Psi_{i,J,m}^{(D)}; \quad i = a, b. \tag{11}$$

NSI amplitude can be found by calculating the following matrix elements:

$$E1_{\rm NSI} = (-1)^{\frac{3}{2}-m} \begin{pmatrix} \frac{3}{2} & 1 & \frac{1}{2} \\ -m & 0 & m \end{pmatrix}^{-1} \tag{12}$$

$$\times \left(\langle \Psi_{6p_{3/2}} | H_{\rm NSI}^{\rm eff} | \Psi_{a,3/2}^{(D)} \rangle + \langle \Psi_{b,1/2}^{(D)} | H_{\rm NSI}^{\rm eff} | \Psi_{6p_{1/2}} \rangle \right),$$

where we skip index m in matrix elements and take advantage of the fact that $H_{\rm NSI}^{\rm eff}$ is diagonal in quantum number J. NSD part of the PNC interaction (3) can change this quantum number, and corresponding amplitudes have more complicated form:

$$E1_{\rm NSD} = \sum_{J=1/2}^{5/2} C(J,F,F') \left(\langle \Psi_{6p_{3/2}} | H_{\rm NSD}^{\rm eff} | \Psi_{a,J}^{(D)} \rangle \right.$$

$$\left. + \ \langle \Psi_{b,J}^{(D)} | H_{\rm NSD}^{\rm eff} | \Psi_{6p_{1/2}} \rangle \right), \tag{13}$$

where constants $C(J,F,F')$ are some combinations of the $6j$-coefficients (see [21] for details).

All wave functions in Eqs. (12), (13) are many-electron ones. In the one-particle approximation, these expressions are simplified, and both NSI and NSD parts of the PNC amplitude have the form:

$$E1_{\rm PNC} = \sum_n \frac{\langle 6p_{3/2} || D || ns_{1/2} \rangle \langle ns_{1/2} | H_{\rm PNC} | 6p_{1/2} \rangle}{\varepsilon_{6p_{1/2}} - \varepsilon_{ns_{1/2}}}. \tag{14}$$

The sum here runs over occupied ($n = 1, \ldots, 6$) and vacant ($n > 6$) states. Contribution of the occupied states with $n \leq 5$ is very small, while $n = 6$ contributes almost as much as the whole sum over vacant states. The term $n = 6$ corresponds to amplitudes with the index b in (12) and (13). It is seen, that all intermediate states in (14) have $J = 1/2$. This leads to the equality $\xi(1,1) = \xi(1,2)$, which is not correct for a more general case of

TABLE I: Calculated values of $\xi(F,F')$ in different approximations: configuration interaction (CI) for three valence electrons, and CI+MBPT method; a and b correspond to two contributions in Eqs. (12) and (13).

	CI			CI+MBPT		
F, F'	a	b	total	a	b	total
0, 1	1.09	1.29	1.20	1.08	1.12	1.10
1, 1	−0.498	−0.513	−0.506	−0.500	−0.431	−0.462
1, 2	−0.337	−0.413	−0.378	−0.331	−0.361	−0.348

Eq. (13). The many-body corrections are strongest for the weak amplitude $F = 1 \to F' = 1$, which affects the value of $\xi(1,1)$.

Our results for the function $\xi(F,F')$ are given in Table 1. We find them from the calculated amplitudes (12) and (13) in two approximations. At first, we use configuration interaction method for three valence electrons with conventional operators. Then, we use second order many-body perturbation theory to construct effective Hamiltonian $H^{\rm eff}$ and random phase approximation for the effective operators $D_z^{\rm eff}$ and $H_{\rm PNC}^{\rm eff}$.

It follows from the comparison of Table 1 with the one-particle approximation (8), that correlation effects enhance NSD amplitudes. For the weakest amplitude $F = 1 \to F' = 1$ the correlation correction exceeds 50%. For two other amplitudes correlations are less important, but still account for 20% – 25% enhancement. Valence correlations are larger for the amplitudes b. The dominant contribution to these amplitudes corresponds to the intermediate states from the configuration $6s6p^2$, where correlations between two p-electrons are very strong. In contrast to that, the main contributions to amplitudes a correspond to configurations $6s^2np$, where correlations are much weaker.

We showed above, that correlation corrections to NSD amplitudes are rather large. Moreover, our values of $\xi(1,1)$ and $\xi(1,2)$ noticeably differ from each other. That leads to the dependence of the experimentally observed amplitude (2b) on x^2. The value of this parameter depends on the experimental conditions. In the linear regime, x^2 and $1-x^2$ are proportional to the intensities of the corresponding lines. That gives $x^2 = \frac{1}{6}$ [19]. Actual experiment [5] was done in the nonlinear regime, when in the center of the line the light was completely absorbed, and PNC signal was detected only on the wings. In these conditions, one can expect that $\frac{1}{6} \le x^2 \le \frac{1}{2}$. Below, we will perform analysis for each of the limiting cases.

If we substitute values from Table 1 to Eq. (7b), we get:

$$\xi(0) = 1.10; \quad \xi(1) = \begin{cases} -0.367, & x^2 = 1/6, \\ -0.405, & x^2 = 1/2. \end{cases} \tag{15}$$

NSI amplitude can be found as weighted average:

$$\mathcal{R}_{\rm NSI} = \frac{\xi(0)\mathcal{R}(1) - \xi(1)\mathcal{R}(0)}{\xi(0) - \xi(1)}\,. \tag{16}$$

Experimental difference between $\mathcal{R}(1)$ and $\mathcal{R}(0)$ is only about 1%. Because of that, both values of $\xi(1)$ from (15) lead to the same value of $\mathcal{R}_{\rm NSI} = -14.68 \times 10^{-8}$ in agreement with the result from [5].

The difference $\Delta\mathcal{R} \equiv \mathcal{R}(1) - \mathcal{R}(0)$ can be written as:

$$\Delta\mathcal{R} = 6\kappa\frac{\xi(0) - \xi(1)}{Q_W}\mathcal{R}_{\rm NSI} \tag{17}$$

$$= -4(\kappa_a + 0.06)\frac{\xi(0) - \xi(1)}{Q_W}\mathcal{R}_{\rm NSI}, \tag{18}$$

where we use relation (5) between κ and κ_a. Table 1 and Eq. (15) give $\xi(0) - \xi(1) = 1.49 \pm 0.02$, and substituting the standard model value $Q_W = -116.7$ [23], we get:

$$\Delta\mathcal{R} = (0.051 \pm 0.001)(\kappa_a + 0.06)\mathcal{R}_{\rm NSI}, \tag{19}$$

where the error bar corresponds to two values of x^2 in (15) and does not account for the theoretical error, caused by the neglect of the higher orders of the many-body perturbation theory. The latter was estimated in [18] for NSI amplitude to be close to 3%. Here we neglect the structural radiation corrections and few other corrections, which can contribute on the percent level, so we estimate the actual accuracy of Eq. (19) to be about 5%. On this level, the uncertainty in experimental conditions described by the parameter x^2 is negligible.

Using experimental values from [5]:

$$\mathcal{R}_{\rm NSI} = (-14.68 \pm 0.06 \pm 0.16) \times 10^{-8}, \tag{20}$$

$$\Delta\mathcal{R} = (0.15 \pm 0.13 \pm 0.15) \times 10^{-8}, \tag{21}$$

we get the following result for the AM constant:

$$\kappa_a = -0.26 \pm 0.27\,. \tag{22}$$

In an independent measurement [11] of PNC effects in Tl a very close central value for the parameter $\Delta\mathcal{R}$ was obtained, though with a three times larger uncertainty. If we use (8) instead of (15), we get $\kappa_a = -0.32 \pm 0.35$. It means, that correlations account for 30% corrections and lead to a smaller absolute value of the AM constant. Note, that in Ref. [5] the approximate values $\xi(0) = 1$ and $\xi(1) = -\frac{1}{3}$ were used instead of the more accurate one-particle values (8), and the relation $\kappa = -\frac{2}{3}\kappa_a$ was used instead of Eq. (5).

It was first recognized by Novikov and Khriplovich [10], that NSD operator also leads to the $E1$-amplitude between hyperfine sublevels of the same electronic state. The most interesting in this respect is the hyperfine transition in the ground state. Such amplitudes were calculated in the one-particle approximation for Cs and Tl [10] and for K [22]. The only many-body calculation was done recently for Fr [21]. It is straitforward to rewrite Eq. (13) for this case, and all calculations are similar to those for optical transition. The result in a.u. is:

$$\langle 6p_{1/2}, 1||E1_{\mathrm{NSD}}||6p_{1/2}, 0\rangle = 2.11 \times 10^{-11}\,\mathrm{i}\,\kappa, \tag{23}$$

where we use the same level of approximation, as above and add normalization correction [18]. In the one-particle approximation the $M1$-amplitude for this transition is equal to $-\frac{\alpha}{2\sqrt{3}}$. Correlations change this value only at sub-percent level, and we can safely use it to calculate $\mathcal{R}$:

$$\begin{aligned} \mathcal{R}_{\mathrm{hf}}(6p_{1/2}) &= -1.00 \times 10^{-8}\,\kappa \\ &= 0.67 \times 10^{-8}(\kappa_a + 0.06). \end{aligned} \tag{24}$$

Comparison of this value with the one obtained in [10] shows that correlations increase the answer by approximately 20%. Result (24) can be compared also to the $F = 4 \rightarrow F' = 5$ transition in the ground state $7s$ of ^{211}Fr, where $\mathcal{R} = 3.0 \times 10^{-9}\kappa$ [21]. Though the $M1$-amplitude for the hyperfine transition in Tl is significantly weaker than in Fr, it should be much easier to do the experiment with stable Tl, than with radioactive Fr. Note, that for lighter Cs, $\mathcal{R}$ is an order of magnitude smaller.

We see that electron correlations account for substantial corrections to AM amplitudes, but do not explain the difference between the experiment [5] and the nuclear theory prediction that $\kappa_a = 0.25 \pm 0.15$ [4]. The experimental accuracy for NSD amplitude for $6p_{1/2} \rightarrow 6p_{3/2}$ transition is not high, because this amplitude is much weaker, than NSI one. Therefore, it may be very interesting to measure the hyperfine amplitude (23), where PNC effects are completely determined by the NSD part of the weak interaction. Note also, that the frequencies of the hyperfine transitions for two natural isotopes ^{203}Tl and ^{205}Tl differ by 1% and should be easily resolved. That gives the possibility to measure AM constants for each of the isotopes.

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