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Manifestation of the Nuclear Anapole Moment in the Thallium *M*1 Transitions[1]

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We calculate the nuclear spin-dependent parity-nonconserving $E1$ amplitudes for the optical transition $6p_{1/2,\,F} \longrightarrow 6p_{3/2,\,F'}$ and hyperfine transition $6p_{1/2,\,F} \longrightarrow 6p_{1/2,\,F'}$ in ^{205}Tl. The experimental limit placed upon the former amplitude by Vetter *et al.* [PRL 74, 2658 (1995)] corresponds to the anapole moment constant $\kappa_a = -0.26 \pm 0.27$. © *2002 MAIK "Nauka/Interperiodica".*

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

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

[1] This article was submitted by the author in English.

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

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

of the PNC amplitude to the magnetic amplitude was measured with an accuracy of 1% in [5] and 3% in [11]. In those experiments, the hyperfine structure of the lower level $6p_{1/2}$ was resolved. This allowed one to determine $\mathcal{R}(F)$ for two ground-state hyperfine levels, $F = 0$ and $F = 1$. For the $F = 0$ level, only the transition to $F' = 1$ of the $6p_{3/2}$ level is allowed, while for the $F = 1$ level the transitions to both upper hyperfine levels $F' = 1, 2$ are allowed. Accordingly, $\mathcal{R}(1)$ is a certain average of 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 the coefficient x^2 depends on the transition intensities and experimental conditions such as the line width and optical depth.

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

$$\begin{aligned} H_{\mathrm{PNC}} &= H_{\mathrm{NSI}} + H_{\mathrm{NSD}} \\ &= \frac{G_F}{\sqrt{2}}\left(-\frac{Q_W}{2}\gamma_5 + \frac{\kappa}{I}\boldsymbol{\alpha}\mathbf{I}\right)\rho(\mathbf{r}), \end{aligned} \tag{3}$$

where $G_F = 2.2225 \times 10^{-14}$ au is the Fermi constant of weak interaction, Q_W is the nuclear weak charge, κ is the dimensionless coupling constant, γ_5 and $\boldsymbol{\alpha} \equiv \gamma_0\boldsymbol{\gamma}$ are the Dirac matrices, I is the nuclear spin ($I = \frac{1}{2}$ for both

stable ^{205}Tl and ^{203}Tl isotopes), and $\rho(\mathbf{r})$ is the nuclear density distribution.

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

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

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

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

Theoretical predictions for the AM constant depend on the 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 the measured values of κ_a to gain information on the coupling constants for the nuclear *P*-odd interaction [14–16].

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

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

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

$$\xi(0) = \xi(0, 1), \quad (7a)$$

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

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 Eqs. (2b) and (7b). Numerical values (obtained in [6]) are

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

In general, when the 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 the function $\xi(F', F)$. After that, the experimental function $\xi(F)$ is given by Eq. (7). Consequently, the difference in the NSI and NSD amplitudes depends on the factor x^2.

The NSI amplitude was studied many times, the most advanced and accurate calculations being performed in [17, 18] (for earlier references, see [19]). It was shown there that the many-body corrections to the PNC amplitudes in Tl may be important. This stimulated us to recalculate the function $\xi(F, F')$. We follow here the same procedure as was used in [18]. It is based on a 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 the basis sets, configuration sets, etc., are the same as in [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. This allowed us to estimate the accuracy of calculation of the NSI amplitude at a level better than 3%. Here, we use the same wave functions for the $6p_j$ states but neglect several smaller corrections (such as structural radiation) to the effective operators for valence electrons. The normalization correction is the same for the NDI and NSD amplitudes and does not affect the function $\xi(F', F)$.

In order to find the PNC amplitude, we solve the inhomogeneous equations

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

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

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

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

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

$$E1_{\rm NSI} = (-1)^{\frac{3}{2}-m}\begin{pmatrix} \frac{3}{2} & 1 & \frac{1}{2} \\ -m & 0 & m \end{pmatrix}^{-1} \times (\langle \Psi_{6p_{3/2}}|H^{\rm eff}_{\rm NSI}|\Psi^{(D)}_{a,3/2}\rangle + \langle \Psi^{(D)}_{b,1/2}|H^{\rm eff}_{\rm NSI}|\Psi_{6p_{1/2}}\rangle), \quad (12)$$

where we omitted the index m in the matrix elements and took advantage of the fact that $H^{\rm eff}_{\rm NSI}$ is diagonal in quantum number J. The NSD part of PNC interaction (3)

[2] Note that the radiative corrections can change κ_2 rather noticeably.

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

F, F'	CI			CI + MBPT		
	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

can change this quantum number, and the corresponding amplitudes have a more complicated form:

$$E1_{\mathrm{NSD}} = \sum_{J=1/2}^{5/2} C(J, F, F') \times (\langle \Psi_{6p_{3/2}} | H^{\mathrm{eff}}_{\mathrm{NSD}} | \Psi^{(D)}_{a,J} \rangle + \langle \Psi^{(D)}_{b,J} | H^{\mathrm{eff}}_{\mathrm{NSD}} | \Psi_{6p_{1/2}} \rangle), \quad (13)$$

where the constants $C(J, F, F')$ are certain combinations of the 6*j* coefficients (see [21] for detail).

All wave functions in Eqs. (12) and (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

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

Here, the sum runs over the occupied ($n = 1, \ldots, 6$) and vacant ($n > 6$) states. The contribution of the occupied states with $n \le 5$ is very small, while $n = 6$ contributes almost as much as the whole sum over the vacant states. The term $n = 6$ corresponds to the amplitudes with index *b* in Eqs. (12) and (13). It can be seen that all intermediate states in Eq. (14) have $J = 1/2$. This leads to the equality $\xi(1, 1) = \xi(1, 2)$, which is incorrect for the more general case of Eq. (13). The many-body corrections are the strongest for the weak $F = 1 \longrightarrow F' = 1$ amplitude, which affects the value of $\xi(1, 1)$.

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

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

We showed above that the correlation corrections to the NSD amplitudes are rather large. Moreover, our values of $\xi(1, 1)$ and $\xi(1, 2)$ noticeably differ from each other. This leads to the dependence of the experimentally observed amplitude (Eq. 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 corresponding line intensities. This gives $x^2 = \frac{1}{6}$ [19]. The actual experiment [5] was done in the nonlinear regime, where the light was completely absorbed at the line center and the PNC signal was detected only at the wings. In these conditions, one can expect that $\frac{1}{6} \le x^2 \le \frac{1}{2}$. Below, we analyze each of the limiting cases.

If we substitute the values from the table into Eq. (7b), we get

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

The NSI amplitude can be found as a weighted average

$$\mathcal{R}_{\mathrm{NSI}} = \frac{\xi(0)\mathcal{R}(1) - \xi(1)\mathcal{R}(0)}{\xi(0) - \xi(1)}. \quad (16)$$

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

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

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

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

where we use relation (5) between κ and κ_a. The table and Eq. (15) give $\xi(0) - \xi(1) = 1.49 \pm 0.02$, and, substituting the standard model value $Q_W = -116.7$ [22], we get

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

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

Using the experimental values from [5],

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

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

we get the following result for the AM constant:

$$\kappa_a = -0.26 \pm 0.27. \qquad (22)$$

In an independent measurement [11] of the PNC effects in Tl, a very close central value for the parameter $\Delta\mathcal{R}$ was obtained, though with an uncertainty that was three times larger. If we use Eq. (8) instead of Eq. (15), we get $\kappa_a = -0.32 \pm 0.35$. This means that the correlations account for 30% of the corrections and lead to a smaller absolute value of the AM constant. Note that in [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 the NSD operator also leads to the $E1$ amplitude between the hyperfine sublevels of the same electronic state. The ground-state hyperfine transition is the most interesting in this respect. The corresponding amplitudes were calculated in the one-particle approximation for Cs and Tl [10] and for K [23]. The only many-body calculation was performed recently for Fr [21]. It is straightforward to recast Eq. (13) for this case, and all the calculations are similar to those for the optical transition. The result in au is

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

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

$$\mathcal{R}_{\rm hf}(6p_{1/2}) = -1.00 \times 10^{-8}\kappa = 0.67 \times 10^{-8}(\kappa_a + 0.06). \qquad (24)$$

Comparison of this value with the one obtained in [10] shows that the correlations increase the result by approximately 20%. Result (24) can also be compared with the $F = 4 \longrightarrow F' = 5$ transition in the ^{211}Fr $7s$ ground state, where $\mathcal{R} = 3.9 \times 10^{-9}\kappa$ [21]. Although the $M1$ amplitude for the hyperfine transition in Tl is significantly smaller than in Fr, it would 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 the electron correlations account for the substantial corrections to the AM amplitudes but do not explain the difference between the experiment [5] and the prediction of nuclear theory that $\kappa_a = 0.25 \pm 0.15$ [4]. The experimental accuracy for the NSD amplitude of the $6p_{1/2} \longrightarrow 6p_{3/2}$ transition is not high, because this amplitude is much smaller, than the NSI amplitude. Therefore, it may be very interesting to measure the hyperfine amplitude (23), where the PNC effects are completely determined by the NSD part of the weak interaction. Note also that the hyperfine transition frequencies for two natural isotopes ^{203}Tl and ^{205}Tl differ by 1% and can be easily resolved. This enables one to measure the AM constants for each of the isotopes.

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