Calculation of the nuclear spin-dependent parity-nonconserving amplitude for the $(7s,F=4)\rightarrow(7s,F=5)$ transition in Fr

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Many-body calculation of nuclear spin-dependent parity-nonconserving amplitude for $7s,F=4\rightarrow 7s,F=5$ transition between hyperfine sublevels of the ground state of ^{211}Fr is carried out. The final result is $\langle 7s,F=5||d_{\rm PNC}||7s,F=4\rangle = -0.49\times 10^{-10}\,i\kappa$ a.u., where κ is the dimensionless coupling constant. This is approximately an order of magnitude larger than similar amplitude in Cs. The dominant contribution to κ is associated with the anapole moment of the nucleus.

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I. INTRODUCTION

In this work we calculated nuclear spin-dependent parity-nonconserving (PNC) amplitude for $7s,F=4\rightarrow 7s,\ F=5$ transition between hyperfine structure components of the ground state of the odd isotope of francium ^{211}Fr. Three effects contribute to this amplitude [1]: the interaction of an electron with the nuclear anapole moment (AM), the electron-nuclear neutral-current interaction, and the combined action of the nuclear spin-independent electron-nucleus weak interaction and the hyperfine interaction.

The AM **a** was introduced by Zel'dovich [2] just after the discovery of parity violation. A first realistic model for the AM of the nucleus was suggested in Refs. [3,4]. There it was shown that for heavy nuclei $a\sim A^{2/3}$, where A is the number of nucleons. AMs of the nuclei with unpaired proton are expected to be few times larger than for the case of unpaired neutron. Because of that for atoms with large and odd Z the AM contribution to the spin-dependent part of the PNC amplitudes dominates over that of the electron-nucleon neutral currents. The third contribution is also $\sim A^{2/3}$, but is numerically smaller [see Eq. (3) below]. Note that the neutral current and hyperfine contributions to the nuclear spin-dependent PNC amplitude are well known from the standard model. Therefore, any measurement of the respective coupling constant κ will give unambiguous information about AM of the nucleus.

For the optical transitions in heavy atoms the spin-independent PNC amplitudes are approximately two orders of magnitude larger than the spin-dependent magnitude. Because of that the AM was measured experimentally only for cesium [7]. This measurement provided a valuable probe of the relatively poorly understood parity nonconservation in nuclei [8,9]. Further experimental and theoretical investigations of AM are very important both for nuclear physics and for physics of the fundamental interactions.

An alternative possibility to observe the spin-dependent PNC amplitudes was suggested in [10]. In the rf transitions between the hyperfine components of the ground state of an atom the spin-independent amplitudes are negligible and the dominant PNC effect is caused by the AM. Using the rf resonator one can have an additional enhancement of the PNC effect by placing the gas cell in the node of the magnetic and the antinode of the electric rf fields [11]. The PNC effect can be also enhanced in the strong dc magnetic field [12]. The cooling and trapping techniques allow to increase the intensity of the rf transitions making these experimental schemes much more realistic. At present there is an ongoing project of measuring PNC effects in francium [13,14] and the observation of the AM in the hyperfine transition can be a valuable addition to this project.

Semiempirical calculations of nuclear spin-dependent amplitudes for transitions between hyperfine sublevels of the ground state were already carried out for Cs and Tl [10] and for K and Cs [11]. Fr is the heaviest of alkali-metal atoms. Since spin-dependent amplitude grows with nuclear charge Z faster than Z^2, one can expect that for Fr this amplitude will be significantly larger than for other alkali-metal atoms. Besides that, a large number of odd isotopes with nonzero nuclear spin makes it possible (at least in principle) to study dependence of nuclear spin-dependent amplitude on the nuclear structure.

II. THEORY

It is known that parity-nonconserving electron-nuclear interaction can be divided into two parts: nuclear spin-independent part and nuclear spin-dependent part. The respective PNC Hamiltonian can be written as follows (atomic units are used throughout the paper):

$$H_{\rm PNC}=H_{\rm SI}+H_{\rm SD}=\frac{G_F}{\sqrt{2}}\left(-\frac{Q_W}{2}\gamma_5+\frac{\kappa}{I}\boldsymbol{\alpha}\mathbf{I}\right)\rho(\mathbf{r}), \qquad (1)$$

where $G_F=2.2225\times 10^{-14}$ a.u. is the Fermi constant of the weak interaction, Q_W is the nuclear weak charge, κ is the dimensionless coupling constant, $\boldsymbol{\alpha}=\gamma_0\boldsymbol{\gamma}$, γ_i are the Dirac matrices, $\mathbf{I}$ is the nuclear spin ($I=\frac{9}{2}$ for the isotope ^{211}Fr), and $\rho(\mathbf{r})$ is the nuclear-density distribution.

As we mentioned above, there are three main contributions to the coupling constant κ in the spin-dependent part of the PNC interaction (1):

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$$\kappa=(-1)^{I+(1/2)-l}\frac{I+\frac{1}{2}}{I+1}\kappa_a+\kappa_2+\kappa_{Q_W}, \tag{2}$$

where the anapole contribution is given by the constant κ_a [3] (l is the orbital angular momentum of the unpaired nucleon), the constant κ_2 corresponds to the spin-dependent weak neutral currents and the term κ_{Q_W} is induced by the interference of the spin-independent PNC interaction with the hyperfine interaction. For heavy nuclei constants κ_a and κ_{Q_W} are proportional to $A^{2/3}$ [5,6], and their ratio depends on the dimensionless constant of the weak interaction of the unpaired nucleon with the nuclear core g [8]

$$\frac{\kappa_{Q_W}}{\kappa_a}\approx q\frac{N\mu_N}{A\mu g}, \tag{3}$$

where μ_N and μ are magnetic moments of the nucleus and the valence nucleon, correspondingly. The numerical factor q is within the limits $1<q<3$ (see, e.g., [8]). For the unpaired proton $g_p\approx 7$, while for neutron $g_n\approx -2$ [8] (see also [9]). This estimate shows that for the odd isotopes of Fr the anapole contribution dominates in Eq. (2).

We assume that the nucleus is a uniformly charged sphere

$$\rho(\mathbf{r})=\frac{3}{4\pi r_n^3}\Theta(r_n-r).$$

The root-mean-square charge radius for ^{211}Fr was measured to be $r_{\rm rms}=5.566$ fm [15]. Using the relation $r_n=\sqrt{(5/3)r_{\rm rms}}$, we find $r_n=7.186$ fm.

If $|i\rangle$ and $|f\rangle$ are initial and final atomic states of the same nominal parity, then to the lowest nonvanishing order, the electric-dipole transition matrix element (ME) is equal to

$$\langle f|d_{q,\rm PNC}|i\rangle=\sum_n\left[\frac{\langle f|d_q|n\rangle\langle n|H_{\rm PNC}|i\rangle}{E_i-E_n}+\frac{\langle f|H_{\rm PNC}|n\rangle\langle n|d_q|i\rangle}{E_f-E_n}\right], \tag{4}$$

where $|a\rangle\equiv|J_a,F_a,M_a\rangle$ and $\mathbf{F}=\mathbf{I}+\mathbf{J}$ is the total angular momentum.

In our case the contribution of $H_{\rm SI}$ [see Eq. (1)] is negligible, so we consider only the nuclear spin-dependent part of the PNC Hamiltonian. The ME of $H_{\rm SD}$ can be written as follows:

$$\langle n|H_{\rm SD}|i\rangle=(-1)^{I+F_i+J_i}\sqrt{I(I+1)(2I+1)}\,\delta_{F_nF_i}\delta_{M_nM_i}\times\begin{Bmatrix}J_n & J_i & 1\\ I & I & F_i\end{Bmatrix}\langle J_n||H_{\rm SD}||J_i\rangle, \tag{5}$$

where $\langle J_n||H_{\rm SD}||J_i\rangle=(G_F/\sqrt{2})(\kappa/I)\langle J_n||\gamma_0\gamma\rho(\mathbf{r})||J_i\rangle$.

The ME of the operator d_q is given by the following expression:

$$\langle f|d_q|n\rangle=(-1)^{F_f-M_f}\begin{pmatrix}F_f & 1 & F_n\\ -M_f & q & M_n\end{pmatrix}\times(-1)^{I+F_n+J_f+1}\sqrt{(2F_n+1)(2F_f+1)}\times\begin{Bmatrix}J_n & J_f & 1\\ F_f & F_n & I\end{Bmatrix}\langle J_f||d||J_n\rangle. \tag{6}$$

Applying the Wigner-Eckart theorem to the PNC amplitude,

$$\langle f|d_{q,\rm PNC}|i\rangle=(-1)^{F_f-M_f}\begin{pmatrix}F_f & 1 & F_i\\ -M_f & q & M_i\end{pmatrix}\times\langle J_f,F_f||d_{\rm PNC}||J_i,F_i\rangle,$$

and substituting Eqs. (5) and (6) in Eq. (4) we get the following expression for the reduced ME of the PNC amplitude:

$$\begin{aligned}\langle J_f,F_f||d_{\rm PNC}||J_i,F_i\rangle&=\sqrt{I(I+1)(2I+1)(2F_i+1)(2F_f+1)}\\&\times\sum_n\left[(-1)^{J_f-J_i}\begin{Bmatrix}J_n & J_i & 1\\ I & I & F_i\end{Bmatrix}\begin{Bmatrix}J_n & J_f & 1\\ F_f & F_i & I\end{Bmatrix}\times\frac{\langle J_f||d||n,J_n\rangle\langle n,J_n||H_{\rm SD}||J_i\rangle}{E_n-E_i}\right.\\&\left.+(-1)^{F_f-F_i}\begin{Bmatrix}J_n & J_f & 1\\ I & I & F_f\end{Bmatrix}\times\begin{Bmatrix}J_n & J_i & 1\\ F_i & F_f & I\end{Bmatrix}\frac{\langle J_f||H_{\rm SD}||n,J_n\rangle\langle n,J_n||d||J_i\rangle}{E_n-E_f}\right].\end{aligned} \tag{7}$$

Note that for the transition between the hyperfine components of the ground state $7s_{1/2}$, one has $J_i=J_f=\frac{1}{2}$, $E_i=E_f=E_{7s}$, and $F_i=F_f-1=I-\frac{1}{2}$. That leads to some simplification of Eq. (7):

$$\begin{aligned}\langle 7s_{1/2},F_f||d_{\rm PNC}||7s_{1/2},F_i\rangle&=2I(I+1)\sqrt{(2I+1)}\\&\times\sum_n\frac{\langle 7s_{1/2}||d||n,J_n\rangle\langle n,J_n||H_{\rm SD}||7s_{1/2}\rangle}{E_n-E_{7s}}\\&\times\left[\begin{Bmatrix}I & I & 1\\ \frac{1}{2} & J_n & F_i\end{Bmatrix}\begin{Bmatrix}F_i & J_n & I\\ \frac{1}{2} & F_f & 1\end{Bmatrix}\right.\\&\left.+\begin{Bmatrix}I & I & 1\\ \frac{1}{2} & J_n & F_f\end{Bmatrix}\begin{Bmatrix}F_f & J_n & I\\ \frac{1}{2} & F_i & 1\end{Bmatrix}\right],\end{aligned} \tag{8}$$

where the sum runs over the states of odd parity with angular momenta $J_n=\frac{1}{2},\frac{3}{2}$. Novikov and Khriplovich pointed out,

that for alkali-atoms contribution of the intermediate states with $J_n=\frac{3}{2}$ is strongly suppressed. If these states are excluded from the sum in Eq. (8), it can be further simplified to the form

$$\langle 7s_{1/2},F_f||d_{\rm PNC}||7s_{1/2},F_i\rangle = \frac{2}{3}\sqrt{I(I+1)(I+\tfrac{1}{2})} \times\sum_n \frac{\langle 7s_{1/2}||d||n,\tfrac{1}{2}\rangle\langle n,\tfrac{1}{2}||H_{\rm SD}||7s_{1/2}\rangle}{E_n-E_{7s}}. \quad (9)$$

Equation (9) was used in the semiempirical calculations [10,11], but here we use the more accurate expression (8).

III. METHOD OF CALCULATIONS AND RESULTS

The Dirac-Fock-Breit equations were solved self-consistently on a radial grid for the core electrons $[1s,\ldots,6p_{3/2}]$. Then, the valence orbitals $7s,7p,8s,8p,9p$ were constructed in V^{N-1} approximation. The basis set used in calculations included also virtual orbitals up to $25s$, $25p$, $24d$, $15f$, and $15g$ formed with the help of the method described in Refs. [16–19].

To find the nuclear spin-dependent PNC amplitude defined by Eq. (8), one needs to sum over intermediate states or solve the corresponding inhomogeneous equations (Sternheimer [20] or Dalgarno-Lewis [21] method). Here we apply the Sternheimer-Dalgarno-Lewis method to the valence part of the problem as described in [18,22]. Solving inhomogeneous equation we find the answer in the Dirac-Fock approximation

$$\langle 7s,\ F=5||d_{\rm PNC}||7s,\ F=4\rangle_{\rm DF}=-0.42\times10^{-10}\,i\kappa\ \text{a.u.} \quad (10)$$

It is known that core-valence correlations usually play an important role for the PNC amplitudes. We first solved the random-phase approximation (RPA) equations, summing a certain sequence of many-body diagrams to all orders for both operators in the right-hand side of Eq. (4). Note that after the RPA equations are solved for the operator $H_{\rm SD}$, the MEs $\langle ns||H_{\rm SD}||np_{3/2}\rangle$ are no longer equal to zero. As a result, the intermediate $np_{3/2}$ states also contribute to the spin-dependent PNC amplitude. We found that their contribution to $\langle 7s,\ F=5||d_{\rm PNC}||7s,\ F=4\rangle$ is about 10%. That contribution is neglected in the approximation (9). The RPA correction changes the PNC amplitude to

$$\langle 7s,\ F=5||d_{\rm PNC}||7s,\ F=4\rangle_{\rm RPA}=-0.48\times10^{-10}\,i\kappa\ \text{a.u.} \quad (11)$$

The core polarization was taken into account by many-body perturbation theory. We completely accounted for the second order of perturbation theory and partly for the higher orders. In particular, we calculated the structural radiation and normalization corrections to the PNC amplitude.

TABLE I. Nuclear spin-dependent PNC amplitude $\langle 7s,F=5||d_{\rm PNC}||7s,F=4\rangle$ in the units $i\times10^{-10}\kappa$. The first column present the result obtained in the Dirac-Fock approximation for the Coulomb-Gaunt potential. Following columns present corrections discussed in the text. In the column MBPT the Brueckner, structural radiation and normalization corrections are summed together. In the column "core" contribution of the core excitations is given.

DFB	+RPA	+MBPT	+"core"	Total
−0.418	−0.058	−0.033	+0.018	−0.491

Finally, taking into account that the initial and final states are the many-electron states one needs to account for the excitations from the np_j shells $(n=2-6)$. It was calculated in Dirac-Fock approximation. Note that the contribution of the core excitations violating Pauli principle is small (see, e.g., [23]) and we neglect it. Respective "core" contribution to the spin-dependent amplitude was estimated to be -3.5%

All mentioned corrections are presented in Table I. Summing them up, we finally obtain

$$\langle 7s,F=5||d_{\rm PNC}||7s,F=4\rangle=-0.49\times10^{-10}\,i\,\kappa\ \text{a.u.} \quad (12)$$

According to Table I the many-body perturbation theory (MBPT) corrections to this amplitude are relatively small. Therefore, we estimate the accuracy of our result to be about few percent.

It is interesting to compare this amplitude to similar amplitudes in K and Cs. The amplitude (8) strongly depends on the nuclear spin I, which is different for all alkalis. Therefore, it is convenient to rewrite it in terms of the matrix element of the electron operator $\boldsymbol{\sigma}=2\mathbf{s}$, as was done in Ref. [11]:

$$\langle 7s,F_f||d_{\rm PNC}||7s,F_i\rangle\equiv iD\kappa\langle F_f||\sigma||F_i\rangle. \quad (13)$$

In this form the parameter D only weakly depends on the nuclear spin I. Combining Eqs. (12) and (13), we get

$$D=10^{-12}\times\begin{cases}-0.07, & \text{for } {}^{39,41}\text{K} \quad [11],\\ -1.4, & \text{for } {}^{133}\text{Cs} \quad [10],\\ -11.0, & \text{for } {}^{211}\text{Fr},\end{cases} \quad (14)$$

where we took into account the differences in definition of the coupling constant κ [26].

One can see that the constant D for Fr is almost an order of magnitude larger, than for Cs. According to the Refs. [24,25], the ratio of the spin-independent PNC amplitudes for optical transitions $ns\to(n+1)s$ for Fr $(n=7)$ and Cs $(n=6)$ is close to 20. That factor also accounts for the 1.6 times difference of the weak charges Q_W in the PNC operator (1) for the two nuclei. Because the interaction of the electron with the nuclear AM gives the main contribution to

the spin-dependent PNC amplitude, one can expect that the constant κ also grows as $A^{2/3}$ [3]. That can account for the extra factor ~ 1.4 for the amplitude (13) in Fr when compared to that in Cs.

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[1] I. B. Khriplovich, *Parity Non-conservation in Atomic Phenomena* (Gordon and Breach, New York, 1991).
[2] Y.B. Zel'dovich, Zh. Eksp. Teor. Fiz. **33**, 1531, (1957) [Sov. Phys. JETP **6**, 1184 (1957)].
[3] V.V. Flambaum and I.B. Khriplovich, Zh. Eksp. Teor. Fiz. **79**, 1656 (1980) [Sov. Phys. JETP **52**, 835 (1980)].
[4] V.V. Flambaum, I.B. Khriplovich, and O.P. Sushkov, Phys. Lett. B **146**, 367 (1984).
[5] V.V. Flambaum and I.B. Khriplovich, Zh. Eksp. Teor. Fiz. **89**, 1505 (1985) [Sov. Phys. JETP **62**, 872 (1985)].
[6] C. Bouchiat and C.A. Piketty, Phys. Lett. B **269**, 195 (1991).
[7] C.S. Wood, S.C. Bennett, D. Cho B.P. Masterson, J.L. Roberts, C.E. Tanner, and C.E. Wieman, Science **275**, 1759 (1997).
[8] V.V. Flambaum and D.W. Murray, Phys. Rev. C **56**, 1641 (1997).
[9] W.C. Haxton and C.E. Wieman, e-print nucl-th/0104026.
[10] V.N. Novikov and I.B. Khriplovich, Pis'ma Zh. Eksp. Teor. Fiz. **22**, 162 (1975) [JETP Lett. **22**, 74 (1975)].
[11] V.G. Gorshkov, V.F. Ezhov, M.G. Kozlov, and A.I. Mikhailov, Yad. Fiz. **48**, 1363 (1988) [Sov. J. Nucl. Phys. **48**, 867 (1988)].
[12] V. V. Flambaum (unpublished).
[13] J.A. Behr, *et al.*, Hyperfine Interact. **81**, 197 (1993).
[14] L.A. Orozco *et al.*, in *First Latin American Symposium on High Energy Physics and VII Mexican School of Particles and Fields*, edited by Juan Carlos D'Olivo, Martin Klein-Kreisler, and Hećtor Méndez, AIP Conf. Proc. No. 400 (AIP, Woodbury, NY 1997) p. 107.
[15] J.S. Grossman, L.A. Orozco, M.R. Pearson, J.E. Simsarian, G.D. Sprouse, and W.Z. Zhao, Phys. Rev. Lett. **83**, 935 (1999).
[16] P. Bogdanovich and G. Žukauskas, Sov. Phys. Collect. **23**, 18 (1983).
[17] P. Bogdanovich, Lith. Phys. J. **31**, 79 (1991).
[18] M.G. Kozlov, S.G. Porsev, and V.V. Flambaum, J. Phys. B **29**, 689 (1996).
[19] M.G. Kozlov and S.G. Porsev, Zh. Éksp. Teor. Fiz. **111**, 831 (1997) [Sov. Phys. JETP **84**, 461 (1997)].
[20] R.M. Sternheimer, Phys. Rev. **80**, 102 (1950).
[21] A. Dalgarno and J.T. Lewis, Proc. R. Soc. Edinburgh, Sect. B: Nat. Environ. **223**, 70 (1955).
[22] M.G. Kozlov and S.G. Porsev, Eur. Phys. J. D **5**, 59 (1999).
[23] M.S. Safronova, W.R. Johnson, and A. Derevianko, Phys. Rev. A **60**, 4476 (1999).
[24] V.A. Dzuba, V.V. Flambaum, and O.P. Sushkov, Phys. Rev. A **51**, 3454 (1995).
[25] M.S. Safronova and W.R. Johnson, Phys. Rev. A **62**, 022112 (2000).
[26] It should be mentioned that several definitions of the coupling constant κ are used in the literature, and one has to take it into account when comparing different results.