Calculation of the parity-violating 5*s*-6*s* *E*1 amplitude in the rubidium atom

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Currently, the theoretical uncertainty limits the interpretation of the atomic parity-nonconservation (PNC) measurements. We calculate the PNC 5*s*-6*s* electric dipole transition amplitude in rubidium and demonstrate that rubidium is a good candidate to search for new physics beyond the standard model since accuracy of the atomic calculations in rubidium can be higher than in cesium. PNC in cesium is currently the best low-energy test of the standard model; therefore, similar measurements for rubidium present a good option for further progress in the field. We also calculate the nuclear spin-dependent part of the PNC amplitude, which is needed for the extraction of the nuclear anapole moment from the PNC measurements.

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I. INTRODUCTION

The study of parity nonconservation in atoms is a low-energy, relatively inexpensive alternative to high-energy searches for new physics beyond the standard model (see, e.g., [1–3]). For example, parity nonconservation in cesium is currently the best low-energy test of the electroweak theory [1,3]. This is due to the high accuracy of the measurements [4] and their interpretation [5] (see also [6–8]). The uncertainty of the measurements is 0.35% [4], while the uncertainty of the calculations is on the level of 0.4%–0.5% [5–7]. This means that the interpretation of the measurements is limited by the accuracy of atomic calculations. The situation is similar for other atoms. For example, the accuracy of the parity-nonconservation (PNC) measurements for thallium is 1% [9], while the accuracy of the calculations is 2.5%–3% [10,11]. It is believed that a good option for further progress may come with the PNC measurements for atoms or ions with electron structure similar to cesium but with higher nuclear charge Z. Higher Z would lead to a larger PNC effect and would probably lead to better accuracy in the measurements. The PNC measurements have been considered for the Ba^+ ion [12,13] and are under progress for the Fr atom [14] and Ra^+ ion [15]. However, the accuracy of the calculations for these systems is unlikely to be better than for cesium. On the contrary, higher Z means larger relativistic effects such as Breit and quantum electrodynamics (QED) corrections, larger uncertainty due to the neutron skin effect, etc. Since the accuracy of the calculations is a limiting factor even for cesium, it does make sense in our view to look in the opposite direction and to consider PNC in rubidium. Rubidium is an alkali atom next to cesium but with smaller Z. The PNC amplitude in rubidium is only seven times smaller than in cesium. Depending on the accuracy of the measurements which can be achieved for rubidium, the study of the PNC in this atom might be a good alternative for further progress in the area.

Rubidium was considered for anapole moment measurements in Ref. [16]. Corresponding atomic calculations were reported in Refs. [17,18]. The calculations of the spin-independent PNC amplitude of the 5*s*-6*s* electric dipole transition in Rb were performed in our early work [10] with 2% accuracy. Only correlation corrections were considered, while Breit, QED, and other small corrections were ignored. In this paper we perform a more detailed analysis of the PNC amplitude in Rb. This includes more accurate treatment of the correlations and a detailed consideration of the Breit, QED, and neutron skin corrections.

II. CALCULATIONS

The Hamiltonian describing parity-nonconserving electron-nucleus interaction can be written as a sum of the nuclear-spin-independent (SI) and the nuclear-spin-dependent (SD) parts (we use atomic units: $\hbar = |e| = m_e = 1$):

$$\hat{H}_{\rm PNC} = \hat{H}_{\rm SI} + \hat{H}_{\rm SD} = \frac{G_F}{\sqrt{2}}\left(-\frac{Q_W}{2}\gamma_5 + \frac{\varkappa}{I}\boldsymbol{\alpha}\boldsymbol{I}\right)\rho(\boldsymbol{r}), \quad (1)$$

where $G_F \approx 2.2225 \times 10^{-14}$ a.u. is the Fermi constant of the weak interaction, Q_W is the nuclear weak charge, $\boldsymbol{\alpha} = \left(\begin{smallmatrix} 0 & \sigma \\ \sigma & 0 \end{smallmatrix}\right)$ and γ_5 are the Dirac matrices, $\boldsymbol{I}$ is the nuclear spin, and $\rho(\mathbf{r})$ is the nuclear density normalized to 1.

Within the standard model the weak nuclear charge Q_W is given by [19]

$$Q_W \approx -0.9877N + 0.0716Z. \quad (2)$$

Here N is the number of neutrons, and Z is the number of protons.

To calculate the PNC amplitude we use the methods developed in our previous works [6,26]. The all-order correlation potential $\hat{\Sigma}$ [27] is used to construct the so-called Brueckner orbitals (BO) for the external electron. BO are found by solving the Hartree-Fock-like equations with an extra operator $\hat{\Sigma}$:

$$(\hat{H}_0 + \hat{\Sigma} - \epsilon_a)\psi_a^{\rm (BO)} = 0. \quad (3)$$

Here $\hat{H}_0$ is the relativistic Hartree-Fock Hamiltonian, and index a numerates valence states. The BO $\psi_a^{\rm (BO)}$ and energy ϵ_a include dominating higher-order correlations. The parity-nonconserving weak interaction as well as the electric dipole interaction of the atom with laser light are included in the framework of the time-dependent Hartree-Fock approximation [26], which is equivalent to the well-known random-phase approximation (RPA).

In the RPA method, a single-electron wave function in external weak and $E1$ fields is

$$\psi = \psi_0 + \delta\psi + Xe^{-i\omega t} + Ye^{i\omega t} + \delta Xe^{-i\omega t} + \delta Ye^{i\omega t}, \quad (4)$$

where ψ_0 is the unperturbed state, $\delta\psi$ is the correction due to weak interaction acting alone, X and Y are corrections due to the photon field acting alone, δX and δY are corrections due to both fields acting simultaneously, and ω is the frequency of the PNC transition. The corrections are found by solving the system of RPA equations self-consistently for the core states

$$\begin{aligned}
(\hat{H}_0-\epsilon_c)\delta\psi_c &= -(\hat{H}_W+\delta\hat{V}_W)\psi_{0c},\\
(\hat{H}_0-\epsilon_c-\omega)X_c &= -(\hat{H}_{E1}+\delta\hat{V}_{E1})\psi_{0c},\\
(\hat{H}_0-\epsilon_c+\omega)Y_c &= -(\hat{H}^\dagger_{E1}+\delta\hat{V}^\dagger_{E1})\psi_{0c},\\
(\hat{H}_0-\epsilon_c-\omega)\delta X_c &= -\delta\hat{V}_{E1}\delta\psi_c-\delta\hat{V}_W X_c-\delta\hat{V}_{E1W}\psi_{0c},\\
(\hat{H}_0-\epsilon_c+\omega)\delta Y_c &= -\delta\hat{V}^\dagger_{E1}\delta\psi_c-\delta\hat{V}_W Y_c-\delta\hat{V}^\dagger_{E1W}\psi_{0c},
\end{aligned} \tag{5}$$

where index c numerates core states, $\hat{H}_W$ is either $\hat{H}_{SI}$ or $\hat{H}_{SD}$ [see Eq. (1)], $\delta\hat{V}_W$ and $\delta\hat{V}_{E1}$ are corrections to the core potential due to the weak and $E1$ interactions, respectively, and $\delta\hat{V}_{E1W}$ is the correction to the core potential due to the simultaneous action of the weak field and the electric field of the photon.

The PNC amplitude between valence states a and b in the RPA approximation is given by

$$\begin{aligned}
E_{\rm PNC} &= \langle\psi_b|\hat{H}_{E1}+\delta\hat{V}_{E1}|\delta\psi_a\rangle+\langle\psi_b|\hat{H}_W+\delta\hat{V}_W|X_a\rangle\\
&\quad+\langle\psi_b|\delta\hat{V}_{E1W}|\psi_a\rangle\\
&= \langle\psi_b|\hat{H}_{E1}+\delta\hat{V}_{E1}|\delta\psi_a\rangle+\langle\delta\psi_b|\hat{H}_{E1}+\delta\hat{V}_{E1}|\psi_a\rangle\\
&\quad+\langle\psi_b|\delta\hat{V}_{E1W}|\psi_a\rangle.
\end{aligned} \tag{6}$$

To include correlations in the calculation of the PNC amplitude one needs to use BO for the valence states a and b in (6). The corrections $\delta\psi_a$ and $\delta\psi_b$ to BO a and b are also found with the use of the correlation potential $\hat{\Sigma}$:

$$(\hat{H}_0-\epsilon_a+\hat{\Sigma})\delta\psi_a = -(\hat{H}_W+\delta\hat{V})\psi_{0a}. \tag{7}$$

Note that the correlation potential $\hat{\Sigma}$ is the energy-dependent operator. To calculate a BO and corrections to it one should use the correlation potential at the energy of this state, i.e., $\hat{\Sigma}\equiv\hat{\Sigma}(\epsilon_a)$ in (3) and (7).

The way to calculate the PNC amplitude described above does not involve direct calculation of the electric dipole transition amplitudes or weak matrix elements or even the energies, apart from the energies of the $5s$ and $6s$ states. However, it is instructive to make comparisons with available experimental data to have an idea of the accuracy of the calculations. For this purpose we have performed the calculations of the energies and magnetic dipole hyperfine-structure constants of the lowest s and $p_{1/2}$ states of Rb as well as the electric dipole transition amplitudes between these states. The calculations are done with the use of the same approach and the same all-order operator $\hat{\Sigma}$ as for the PNC calculations [28]. The results for the energies and the hyperfine structure are presented in Table I, results for E1 transition amplitudes are given in Table II. Comparison with experimental data shows that the accuracy of the calculations is about 0.1% for the energies, 0.4%–0.6% for the hyperfine structure (hfs) and about 0.3% for the $E1$ transition amplitudes. If we assume that the square root of the product of hfs constants of s and p states can be used as a test for the weak matrix elements ($\langle s|W|p\rangle\sim\sqrt{A_sA_p}$), then the accuracy for the weak matrix elements is also on the level of 0.3%. Note, however, that the accuracy of this test is limited.

TABLE I. Ionization energies and hyperfine-structure constants A for low states of ^{85}Rb.

State	Energies (cm^{-1})		A (MHz)	
	Expt.[a]	Calc.	Expt.	Calc.
$5s_{1/2}$	33691	33666	1011.9[b]	1016
$5p_{1/2}$	21113	21145	120.5[c]	120.1
$5p_{3/2}$	20874	20902		
$4d_{3/2}$	14336	14362		
$4d_{5/2}$	14335	14360		
$6s_{1/2}$	13558	13509	239.18(3)[d]	239.2
$6p_{1/2}$	9976	9973	39.11(3)[e]	38.87
$6p_{3/2}$	9898	9894		

[a]Reference [20].
[b]Reference [21].
[c]Reference [22].
[d]Reference [23].
[e]Reference [24].

For example, the value of the ratio $\langle s|W|p\rangle/\sqrt{A_sA_p}$ is 4% different in Hartree-Fock and RPA approximations. This is because core polarization effects are significantly different for weak and hfs interactions. Only s and $p_{1/2}$ states contribute to the core polarization for the weak matrix elements. In the case of hfs interaction the $p_{3/2}$ states also give a significant contribution. Since weak matrix elements are simpler, the accuracy for them is expected to be higher than for the hyperfine structure.

III. RESULTS AND DISCUSSION

The value of the spin-independent PNC amplitude for the $5s$–$6s$ transition in ^{87}Rb (without Breit, QED, and neutron skin corrections) is

$$|E_{\rm PNC}| = 1.400\times10^{-12}ea_B(-Q_W/N). \tag{8}$$

This is in very good agreement with the value

$$|E_{\rm PNC}| = 1.39(2)\times10^{-12}ea_B(-Q_W/N)$$

presented in our early calculations [10].

Below we will discuss and compare different contributions to the spin-independent PNC amplitudes in rubidium and cesium and point to some advantages of using rubidium in searching for new physics beyond the standard model. The contributions are presented in Table III. We use the ^{87}Rb isotope as an example.

a. Correlations. The total correlation correction to the PNC amplitude is small for both atoms. It is 2% for cesium and 4% for rubidium. The small value of the correlation correction is the result of strong cancellation between different terms.

TABLE II. Electric dipole transition amplitudes (reduced matrix elements in a.u.) for low states of Rb.

Transitions	Expt.[a]	Calc.
$5s_{1/2}$-$5p_{1/2}$	4.231(3)	4.246
$5s_{1/2}$-$5p_{3/2}$	5.977(4)	5.994

[a]Reference [25].

TABLE III. Contributions to the parity-nonconserving electric dipole transition 5s-6s in ^{87}Rb and 6s-7s in ^{133}Cs $[10^{-12} iea_B(-Q_W/N)]$.

	Rb		Cs	
Contribution	a.u.	%	a.u.	%
RPA	1.345	97%	8.899	99%
Correlations	0.054	4%	0.173	2%
Subtotal	1.400	101%	9.072	101%
Breit	− 0.006	− 0.4%	− 0.055	− 0.6%
QED	− 0.003	− 0.2%	− 0.029	− 0.3%
Neutron skin	− 0.0008	− 0.06%	− 0.018	− 0.2%
Total	1.390	100%	8.970	100%

This is illustrated by the data in Table IV, where correlation corrections are presented for each term in (6). In Table IV we use the notation $\tilde{d} = \hat{H}_{E1} + \delta\hat{V}_{E1}$ for short. The largest correlation corrections are for those terms which have $\delta\psi$ weak correction to the ground state. Corresponding corrections for Rb are larger than for Cs. Indeed, the closer the valence electron is to the core, the larger the correlation correction is. The ionization potential for Rb is larger than for Cs. This means that the valence electron in Rb is closer to the core than in Cs. Also, the cancellation between the contributions of $\delta\psi_a$ and $\delta\psi_b$ in Rb is not as strong as in Cs.

Note that the strong cancellations between correlation corrections to different terms in (6) do not mean poor numerical accuracy. The theoretical uncertainty of the PNC amplitudes is mostly due to missed terms, while the numerical accuracy for all terms in (6) is high.

Table IV does not include non-Brueckner correlation corrections, such as structure radiation, weak correlation potential, and renormalization of the wave functions [6]. These corrections are suppressed by a small parameter $E_{\rm valence}/E_{\rm core} \sim 1/10$, where $E_{\rm valence}$ and $E_{\rm core}$ are typical excitation energies of the valence and core electrons. Moreover, their total contribution is practically zero for Cs [6] due to cancellation between different terms. It is expected to be very small for Rb as well since all other relative contributions to E_{PNC} in Rb and Cs are similar. These terms can be calculated

TABLE IV. Correlation corrections Δ to the PNC amplitude, with a comparison between rubidium and cesium. Units are $10^{-12} iea_B(-Q_W/N)$. Indices a and b stand for 7s and 6s for Cs and for 6s and 5s for Rb.

Approximation	$\langle\delta\psi_a\vert\tilde{d}\vert\psi_b\rangle$	$\langle\psi_a\vert\tilde{d}\vert\delta\psi_b\rangle$	$\langle\psi_a\vert\delta\hat{V}_{E1W}\vert\psi_b\rangle$	Total
		Cesium		
RPA	− 3.041	11.965	− 0.0249	8.899
BO[a]	− 3.358	12.454	− 0.0242	9.072
Δ	− 0.316	0.489	− 0.001	0.173
Δ (%)	− 3.5%	5.4%	0.0%	2.0%
		Rubidium		
RPA	− 0.408	1.756	− 0.003	1.345
BO[a]	− 0.463	1.866	− 0.003	1.400
Δ	− 0.055	0.011	0.000	0.055
Δ (%)	− 3.9%	7.8%	0.0%	4.0%

[a]Brueckner orbitals with core polarization.

if progress is made with the measurements. At the moment we just assume that they do not contribute to the PNC amplitude or its uncertainty.

The data in Table IV show that the correlation correction to the PNC amplitudes are similar in cesium and rubidium. Therefore, similar uncertainty is expected. The uncertainty for cesium is 0.4% – 0.5% [5,6]. It is natural to expect the same uncertainty for rubidium.

b. Breit interaction. In was demonstrated in [29] that Breit interaction gives a significant contribution to the PNC in many-electron atoms. The contribution of Breit interaction is about −0.6% to the PNC amplitude in Cs [29,30] (see also Table III). To calculate Breit correction in Rb we use the same approach as in our previous works [30,31]. The Breit Hamiltonian includes magnetic and retardation terms. The Coulomb interaction everywhere in the calculations is replaced by the sum of Coulomb and Breit terms $V \to V_C + V_B$. The second-order correlation correction operator $\hat{\Sigma}$ is used to calculate Brueckner orbitals. The correction is found as a difference between two results for Eq. (6), one with the Breit interaction included and another when it is not included. The resulting Breit correction is about −0.4% of the PNC amplitude in Rb. Its relative value is about 1.5 times smaller than in Cs. Therefore, the uncertainty associated with this correction is also smaller for Rb than for Cs.

c. QED corrections. The quantum electrodynamics corrections to the E_{PNC} for rubidium are calculated using the sum-over-states method. The sum which needs to be evaluated is

$$E_{\rm PNC} = \sum_n \left[\frac{\langle 6s|\tilde{d}|np_{1/2}\rangle\langle np_{1/2}|\tilde{H}_W|5s\rangle}{E_{5s} - E_{np}} + \frac{\langle 6s|\tilde{H}_W|np_{1/2}\rangle\langle np_{1/2}|\tilde{d}|5s\rangle}{E_{6s} - E_{np}} \right]. \quad (9)$$

Here the tilde means that core polarization is taken into account (e.g., $\tilde{d} = \hat{H}_{E1} + \delta\hat{V}_{E1}$). Correlations are taken into account by using Brueckner orbitals for all ns and $np_{1/2}$ states.

We have considered three QED contributions to the PNC amplitude: the corrections to energy denominators, $E1$ dipole matrix elements ($\tilde{d}$), and weak-interaction matrix elements ($\tilde{H}_W$). Corrections to the weak matrix elements have been considered previously [32,33] (see also [34]). From these works, we determine the QED contribution to the PNC amplitude coming from corrections to the weak matrix elements to be −0.30(2)%.

For the corrections coming from the energy denominators and dipole amplitudes, we use the "radiative potential" method proposed in [8]. By calculating the dominating terms in Eq. (9) both with and without QED corrections, we determine the correction coming from the energy denominators to be −0.25% and from the dipole amplitudes to be +0.31%, giving a combined shift of +0.06(3)% for dipoles and energies.

Therefore, we find the total QED shift to the 5s-6s PNC amplitude in rubidium to be −0.24(4)%. As expected, the Rb result is smaller than that in the Cs atom. More importantly, omitted higher-order corrections in $Z\alpha$ should be much smaller in Rb.

d. Neutron skin. The neutron skin correction to the PNC amplitude is due to the fact that nuclear density in the weak

interaction Hamiltonian (1) is not the same as nuclear charge distribution. This density is dominated by neutrons, and if the neutron distribution radius differs from the radius of the proton distribution, this would lead to a correction to the PNC amplitude. It was found from an analysis of data for antiprotonic atoms [35] that the root-mean-square radii of the proton and neutron distributions differ by

$$\Delta r_{np} = (-0.04 \pm 0.03) + (1.01 \pm 0.15)\frac{N-Z}{A}\ \text{fm}. \qquad (10)$$

Using these data to correct nuclear density in (1) and recalculating the PNC amplitude lead to -0.2% correction for Cs and -0.06% correction for Rb (see Table III). Here again the correction is much smaller for Rb than for Cs, leading to smaller uncertainty in the PNC amplitude.

Combining all corrections, we obtain the final value of the $5s$-$6s$ nuclear-spin-independent PNC amplitude in ^{87}Rb,

$$|E_{\rm PNC}| = 1.390(7) \times 10^{-12} e a_B (-Q_W/N), \qquad (11)$$

and for ^{85}Rb,

$$|E_{\rm PNC}| = 1.333(7) \times 10^{-12} e a_B (-Q_W/N). \qquad (12)$$

We assume the 0.5% uncertainty as has been discussed above.

The nuclear spin-dependent PNC amplitudes for transitions between different hyperfine-structure components of the $5s$ and $6s$ states of ^{85}Rb and ^{87}Rb are presented in Table V. They are calculated using the same approximation as for the spin-independent PNC amplitudes, constructing Brueckner orbitals with the use of the all-order correlation potential $\hat{\Sigma}$ and the RPA method for the core polarization. Therefore, the same uncertainty of 0.5% is assumed.

TABLE V. PNC amplitudes (z components) for the $|5s, F_1\rangle \to |6s, F_2\rangle$ transitions in ^{85}Rb and ^{87}Rb. Units are $10^{-11} i e a_0$. The uncertainty is 0.5%.

Isotope	Q_W	I	F_1	F_2	PNC amplitude
^{85}Rb	−44.76	2.5	2	2	$0.0911(5)[1 + 0.1533(8)\varkappa]$
			2	3	$-0.1018(5)[1 - 0.2063(10)\varkappa]$
			3	2	$-0.1018(5)[1 + 0.2501(13)\varkappa]$
			3	3	$-0.1366(7)[1 - 0.1095(5)\varkappa]$
^{87}Rb	−46.74	1.5	1	1	$0.0713(4)[1 + 0.1049(5)\varkappa]$
			1	2	$-0.1235(6)[1 - 0.1247(6)\varkappa]$
			2	1	$-0.1235(6)[1 + 0.1667(8)\varkappa]$
			2	2	$-0.1426(7)[1 - 0.0629(3)\varkappa]$

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