QED corrections to the parity-nonconserving $6s$-$7s$ amplitude in ^{133}Cs

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The complete gauge-invariant set of the one-loop QED corrections to the parity-nonconserving $6s$-$7s$ amplitude in ^{133}Cs is evaluated to all orders in αZ using a local version of the Dirac-Hartree-Fock potential. The calculations are peformed in both length and velocity gauges for the absorbed photon. The total binding QED correction is found to be -0.27(3)%. The weak charge of ^{133}Cs, derived using two most accurate values of the vector transition polarizability β, is $Q_W = -72.57(46)$ for $\beta = 26.957(51)a_{\rm B}^3$ and $Q_W = -73.09(54)$ for $\beta = 27.15(11)a_{\rm B}^3$. The first value deviates by 1.1σ from the prediction of the Standard Model, while the second one is in perfect agreement with it.

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Investigations of parity noncoservation (PNC) effects in atomic systems play a prominent role in tests of the Standard Model (SM) and impose constraints on physics beyond it [1, 2]. The $6s$-$7s$ PNC amplitude in ^{133}Cs [3] remains one of the most attractive subject for such investigations. The measurement of this amplitude to a 0.3% accuracy [4, 5] has stimulated a reanalysis of related theoretical contributions. First, it was found [6–9] that the role of the Breit interaction had been underestimated in previous evaluations of this effect [10, 11]. Then, it was pointed out [12] that the QED corrections may be comparable with the Breit corrections. The numerical evaluation of the vacuum-polarization (VP) correction [13] led to a 0.4% increase of the $6s$-$7s$ PNC amplitude in ^{133}Cs, which resulted in a 2.2σ deviation of the weak charge of ^{133}Cs from the SM prediction. This has triggered a great interest to calculations of the one-loop QED corrections to the PNC amplitude.

While the VP contribution can easily be evaluated to a high accuracy within the Uehling approximation, the calculation of the self-energy (SE) contribution is a much more demanding problem (here and below we imply that the SE term embraces all one-loop vertex diagrams as well). To zeroth order in αZ, it was derived in Refs. [14, 15]. This correction, whose relative value equals to $-\alpha/(2\pi)$, is commonly included in the definition of the nuclear weak charge. The αZ-dependent part of the SE correction to the PNC matrix element between s and p states was evaluated in Refs. [16, 17]. These calculations, which are exact to first order in αZ and partially include higher-order binding effects, yield the correction of -0.9(1)% [16, 18] and -0.85% [17]. This restored the agreement with SM.

Despite of the close agreement of the results obtained in Refs. [17, 18], the status of the QED correction to PNC in ^{133}Cs cannot be considered as resolved until a complete αZ-dependence calculation of the SE correction to the $6s$-$7s$ transition amplitude is accomplished. The reasons for that are the following. First, in case of cesium ($Z = 55$) the parameter $\alpha Z \approx 0.4$ is not small and, therefore, the higher-order corrections can be significant. Second, because the calculations [16–18] are performed for the PNC matrix element only, they do not include other SE diagrams which contribute to the $6s$-$7s$ transition amplitude. For instance, these calculations do not account for diagrams in which the virtual photon embraces both the weak interaction and the absorbed photon. Our calculations, however, show that the contributions of all diagrams are of the same order of magnitude (in both length and velocity gauges, see below), and the final result arises through a delicate cancellation of individual terms, none of which can be neglected. Third, strictly speaking, the PNC matrix element between the states of different energies is not gauge invariant. Despite the gauge-dependent part is suppressed by the small energy difference [17], estimates of the uncertainty in the definition of the PNC diagrams may fail due to unphysical origin of the gauge-dependent terms.

The first step towards a complete αZ-dependence calculation was done in Ref. [19], where the SE correction to the $2s$-$2p_{1/2}$ PNC transition in H-like ions was evaluated. This transition was chosen to deal with the simplified gauge-invariant amplitude. The results of that work agree with those of Refs. [16–18]. However, as was stressed there, no claims can be made about the applicability of these results to the $6s$-$7s$ PNC transition in neutral cesium. In this Letter we calculate the whole gauge-invariant set of the one-loop QED corrections to the $6s$-$7s$ PNC transition amplitude in ^{133}Cs and compare the obtained result with the previous treatments.

A systematic derivation of the QED corrections in a fully relativistic approach requires the use of perturbation theory starting with a one-electron approximation in an effective local potential $V(r)$. In neutral atoms, it is natural to assume that $V(r)$ includes not only the Coulomb field of the nucleus but also a part of the electron-electron interaction. The interaction of the electrons with the quantized electromagnetic field and the correlation effects are accounted for by perturbation theory. In this way we obtain quantum electrodynamics in the Furry picture.

To derive formal expressions for the transition amplitude we employ the method developed in Ref. [20] and described in detail in Ref. [21]. Since the wave length of the absorbed photon is much larger than the atomic size, one can use the dipole approximation. Within this approximation, calculations in the velocity gauge are performed using formulas given

in Ref. [21] with the replacement $\exp(i\mathbf{k}\cdot\mathbf{x}) \to 1$ in the photon wave function. The corresponding formulas in the length gauge are easily obtained by replacing $\boldsymbol{\alpha}$ with $\mathbf{r}$ in all vertices corresponding to the photon absorbtion and by multiplying the amplitude with the factor $i(E_b - E_a)$, where E_a and E_b are the total energies of the atom in the initial ($6s$) and final ($7s$) states, respectively. This simple rule can be derived using Eq. (205) of Ref. [21] and the equal-time commutation relations.

To zeroth order, the $6s$-$7s$ PNC transition amplitude, which is usually employed in these calculations, is

$$E_{\rm PNC} = \sum_n \Big[\frac{\langle b|d_z|n\rangle\langle n|H_W|a\rangle}{\varepsilon_a - \varepsilon_n} + \frac{\langle b|H_W|n\rangle\langle n|d_z|a\rangle}{\varepsilon_b - \varepsilon_n} \Big] . \quad (1)$$

Here a and b denote the $6s$ and $7s$ one-electron states, respectively, with the angular momentum projections $m_a = m_b = 1/2$, $d_z = ez$ is the z projection of the dipole moment operator ($e < 0$), $H_W = -(G_F/\sqrt{8})Q_W \rho_{\rm nuc}(r)\gamma_5$ is the nuclear spin-independent weak-interaction Hamiltonian [1], G_F is the Fermi constant, γ_5 is the Dirac matrix, and $\rho_{\rm nuc}$ is the weak-charge distribution. The one-loop SE corrections are defined by diagrams presented in Fig. 1. The derivation of the formulas for these diagrams is very similar to that for the QED corrections to the transition amplitude described in detail in Ref. [21]. As a result, the SE correction is given by the sum of the following terms:

$$\begin{aligned}\delta E^{\rm a}_{\rm PNC} &= \sum_{n_1,n_2}^{(n_1\neq b)} \frac{\langle b|\Sigma(\varepsilon_b)|n_1\rangle\langle n_1|d_z|n_2\rangle\langle n_2|H_W|a\rangle}{(\varepsilon_b - \varepsilon_{n_1})(\varepsilon_a - \varepsilon_{n_2})} \\ &+ \frac{1}{2}\sum_n \frac{\langle b|\Sigma'(\varepsilon_b)|b\rangle\langle b|d_z|n\rangle\langle n|H_W|a\rangle}{(\varepsilon_a - \varepsilon_n)} , \quad (2)\end{aligned}$$

$$\begin{aligned}\delta E^{\rm b}_{\rm PNC} &= \sum_{n_1,n_2}^{(n_2\neq a)} \frac{\langle b|H_W|n_1\rangle\langle n_1|d_z|n_2\rangle\langle n_2|\Sigma(\varepsilon_a)|a\rangle}{(\varepsilon_b - \varepsilon_{n_1})(\varepsilon_a - \varepsilon_{n_2})} \\ &+ \frac{1}{2}\sum_n \frac{\langle b|H_W|n\rangle\langle n|d_z|a\rangle\langle a|\Sigma'(\varepsilon_a)|a\rangle}{(\varepsilon_b - \varepsilon_n)} , \quad (3)\end{aligned}$$

$$\begin{aligned}\delta E^{\rm c}_{\rm PNC} &= \sum_{n_1,n_2}^{(n_1\neq b)} \frac{\langle b|\Sigma(\varepsilon_b)|n_1\rangle\langle n_1|H_W|n_2\rangle\langle n_2|d_z|a\rangle}{(\varepsilon_b - \varepsilon_{n_1})(\varepsilon_b - \varepsilon_{n_2})} \\ &+ \frac{1}{2}\sum_n \frac{\langle b|\Sigma'(\varepsilon_b)|b\rangle\langle b|H_W|n\rangle\langle n|d_z|a\rangle}{(\varepsilon_b - \varepsilon_n)} \\ &- \sum_n \frac{\langle b|\Sigma(\varepsilon_b)|b\rangle\langle b|H_W|n\rangle\langle n|d_z|a\rangle}{(\varepsilon_b - \varepsilon_n)^2} , \quad (4)\end{aligned}$$

$$\begin{aligned}\delta E^{\rm d}_{\rm PNC} &= \sum_{n_1,n_2}^{(n_2\neq a)} \frac{\langle b|d_z|n_1\rangle\langle n_1|H_W|n_2\rangle\langle n_2|\Sigma(\varepsilon_a)|a\rangle}{(\varepsilon_a - \varepsilon_{n_1})(\varepsilon_a - \varepsilon_{n_2})} \\ &+ \frac{1}{2}\sum_n \frac{\langle b|d_z|n\rangle\langle n|H_W|a\rangle\langle a|\Sigma'(\varepsilon_a)|a\rangle}{(\varepsilon_a - \varepsilon_n)} \\ &- \sum_n \frac{\langle b|d_z|n\rangle\langle n|H_W|a\rangle\langle a|\Sigma(\varepsilon_a)|a\rangle}{(\varepsilon_a - \varepsilon_n)^2} , \quad (5)\end{aligned}$$

$$\delta E^{\rm e}_{\rm PNC} = \sum_{n_1,n_2} \frac{\langle b|d_z|n_1\rangle\langle n_1|\Sigma(\varepsilon_a)|n_2\rangle\langle n_2|H_W|a\rangle}{(\varepsilon_a - \varepsilon_{n_1})(\varepsilon_a - \varepsilon_{n_2})} , \quad (6)$$

$$\delta E^{\rm f}_{\rm PNC} = \sum_{n_1,n_2} \frac{\langle b|H_W|n_1\rangle\langle n_1|\Sigma(\varepsilon_b)|n_2\rangle\langle n_2|d_z|a\rangle}{(\varepsilon_b - \varepsilon_{n_1})(\varepsilon_b - \varepsilon_{n_2})} , \quad (7)$$

$$\begin{aligned}\delta E^{\rm g}_{\rm PNC} &= \frac{i}{2\pi}\int_{-\infty}^{\infty} d\omega \sum_{n,n_1,n_2} \frac{\langle n_1|d_z|n_2\rangle\langle n|H_W|a\rangle}{(\varepsilon_a - \varepsilon_n)} \\ &\times \frac{\langle bn_2|I(\omega)|n_1 n\rangle}{[\varepsilon_b - \omega - u\varepsilon_{n_1}][\varepsilon_a - \omega - u\varepsilon_{n_2}]} , \quad (8)\end{aligned}$$

$$\begin{aligned}\delta E^{\rm h}_{\rm PNC} &= \frac{i}{2\pi}\int_{-\infty}^{\infty} d\omega \sum_{n,n_1,n_2} \frac{\langle b|H_W|n\rangle\langle n_1|d_z|n_2\rangle}{(\varepsilon_b - \varepsilon_n)} \\ &\times \frac{\langle nn_2|I(\omega)|n_1 a\rangle}{[\varepsilon_b - \omega - u\varepsilon_{n_1}][\varepsilon_a - \omega - u\varepsilon_{n_2}]} , \quad (9)\end{aligned}$$

$$\begin{aligned}\delta E^{\rm i}_{\rm PNC} &= \frac{i}{2\pi}\int_{-\infty}^{\infty} d\omega \sum_{n,n_1,n_2} \frac{\langle n_1|H_W|n_2\rangle\langle n|d_z|a\rangle}{(\varepsilon_b - \varepsilon_n)} \\ &\times \frac{\langle bn_2|I(\omega)|n_1 n\rangle}{[\varepsilon_b - \omega - u\varepsilon_{n_1}][\varepsilon_b - \omega - u\varepsilon_{n_2}]} , \quad (10)\end{aligned}$$

$$\begin{aligned}\delta E^{\rm j}_{\rm PNC} &= \frac{i}{2\pi}\int_{-\infty}^{\infty} d\omega \sum_{n,n_1,n_2} \frac{\langle b|d_z|n\rangle\langle n_1|H_W|n_2\rangle}{(\varepsilon_a - \varepsilon_n)} \\ &\times \frac{\langle nn_2|I(\omega)|n_1 a\rangle}{[\varepsilon_a - \omega - u\varepsilon_{n_1}][\varepsilon_a - \omega - u\varepsilon_{n_2}]} , \quad (11)\end{aligned}$$

$$\begin{aligned}\delta E^{\rm k}_{\rm PNC} &= \frac{i}{2\pi}\int_{-\infty}^{\infty} d\omega \sum_{n_1,n_2,n_3} \frac{\langle bn_2|I(\omega)|n_1 a\rangle}{[\varepsilon_b - \omega - u\varepsilon_{n_1}]} \\ &\times \frac{\langle n_1|d_z|n_3\rangle\langle n_3|H_W|n_2\rangle}{[\varepsilon_a - \omega - u\varepsilon_{n_3}][\varepsilon_a - \omega - u\varepsilon_{n_2}]} , \quad (12)\end{aligned}$$

$$\begin{aligned}\delta E^{\rm l}_{\rm PNC} &= \frac{i}{2\pi}\int_{-\infty}^{\infty} d\omega \sum_{n_1,n_2,n_3} \frac{\langle bn_2|I(\omega)|n_1 a\rangle}{[\varepsilon_b - \omega - u\varepsilon_{n_1}]} \\ &\times \frac{\langle n_1|H_W|n_3\rangle\langle n_3|d_z|n_2\rangle}{[\varepsilon_b - \omega - u\varepsilon_{n_3}][\varepsilon_a - \omega - u\varepsilon_{n_2}]} . \quad (13)\end{aligned}$$

Here the SE operator is defined by

$$\langle c|\Sigma(E)|d\rangle \equiv \frac{i}{2\pi}\int_{-\infty}^{\infty} d\omega \sum_n \frac{\langle cn|I(\omega)|nd\rangle}{E - \omega - u\varepsilon_n} , \quad (14)$$

$I(\omega) \equiv e^2\alpha^\mu\alpha^\nu D_{\mu\nu}(\omega)$, $\alpha^\mu \equiv \gamma^0\gamma^\mu = (1, \boldsymbol{\alpha})$, $D_{\mu\nu}(\omega)$ is the photon propagator defined as in Ref. [21], $\Sigma'(E) = d\Sigma(E)/dE$, and $u = 1 - i0$ ensures the correct position of poles of the electron propagators with respect to the integration contour. Taking into account the corresponding diagrams with the mass counterterm results in the replacement

TABLE I: The binding energies of low-lying states in Cs, in a.u.

State	Loc. pot.	DHF	Exp.
$6s_{1/2}$	-0.13079	-0.12824	-0.14310
$6p_{1/2}$	-0.08696	-0.08582	-0.09217
$7s_{1/2}$	-0.05621	-0.05537	-0.05865
$7p_{1/2}$	-0.04251	-0.04209	-0.04393

$\Sigma(E) \to \Sigma(E) - \gamma^0\delta m$. The expressions for the VP corrections, which do not contain any insertions with the external photon line or the weak interaction attached to the electron loop, are obtained from Eqs. (2)-(7) by the replacement of the SE operator with the VP potential. The other VP corrections will not be considered here, since their contribution is negligible.

The corresponding expressions in the velocity gauge are obtained by the replacement $d_z \to -ie\alpha_z/(E_b - E_a)$, where the energies E_a and E_b include the QED corrections. In addition to the replacement $d_z \to -ie\alpha_z/(\varepsilon_b - \varepsilon_a)$ in Eqs. (1)-(13), it yields the contribution

$$\delta E^{\rm add}_{\rm PNC} = -\frac{\langle b|\Sigma(\varepsilon_b)|b\rangle - \langle a|\Sigma(\varepsilon_a)|a\rangle}{\varepsilon_b - \varepsilon_a} E_{\rm PNC}\,, \qquad (15)$$

which results from the expansion of the factor $1/(E_b - E_a)$.

Formulas (2)-(15) contain ultraviolet and infrared divergences. To cancel the ultraviolet divergences, we expand contributions (2)-(7) into zero-, one-, and many-potential terms and contributions (8)-(11) into zero- and many-potential terms. The ultraviolet divergencies are present only in the zero- and one-potential terms. They are removed analytically by calculating these terms in the momentum space (for details, we refer to Refs. [22–24]). The many-potential terms are evaluated in configuration space. The infrared divergences, which occur in contributions (2)-(5) and (12)-(13), are regularized by introducing a nonzero photon mass and cancelled analytically.

Since the levels $6s$, $6p_{1/2}$, $7s$, and $7p_{1/2}$ are very close to each other, to get reliable results for the transition amplitude under consideration, one needs to use a local potential $V(r)$ that reproduces energies and wave functions of these states on the Dirac-Hartree-Fock (DHF) accuracy level or better. We construct such a potential by inverting the radial Dirac equation with the radial wave function obtained by solving the DHF equation with the code of Ref. [25]. Details of this procedure will be published elsewhere. In Table 1, we compare the energies obtained with the local potential $V(r)$, that was derived using mainly the DHF wave function of the $6s$ state, with the DHF energies and with the experimental ones.

Numerical evaluation of expressions (1)-(15) was performed by employing the dual-kinetic-balance finite basis set method [26] with basis functions construced from B-splines. The calculation of the zeroth-order contribution, with $V(r)$ constructed as indicated above, yields $E_{\rm PNC}$ =-1.002, in units $\mathrm{i}\times 10^{-11} Q_W/(-N)$ a.u. This value should be compared with the corresponding DHF value, -0.742 [7], and with the value that includes the correlation effects, -0.908 [10]. The results for the SE corrections are presented in Table 2. Since there is a significant cancellation between terms containing the infrared singularities, the terms corresponding to $n = a$ in $\Sigma'(\varepsilon_a)$ and $n = b$ in $\Sigma'(\varepsilon_a)$ are subtracted from contributions (2)-(5) and added to contributions (12)-(13). The total SE correction $\delta E^{\rm tot}_{\rm PNC}$ contains also the free term, $-\alpha/(2\pi)E_{\rm PNC}$, mentioned above. Since this term is usually included into the weak charge Q_W, one has to consider the binding SE correction defined as $\delta E^{\rm bind}_{\rm PNC} = \delta E^{\rm tot}_{\rm PNC} + \alpha/(2\pi)E_{\rm PNC}$. According to Table 2, the binding SE correction amounts to -0.67%. To estimate the uncertainty of this value due to correlation effects, we have also performed the calculations with $V(r)$ constructed employng the DHF wave function of the $7s$ state. While this leads to a 2% decrease of the transition amplitude, the relative shift of the SE correction is five times smaller. Since the correlation effects contribute to the transition amplitude on the 20% level, we assume a 4% uncertainty for the total SE correction. Therefore, our value for the binding SE correction is -0.67(3)%. This value differs from the previous evaluations of the SE effect, -0.9(1)% [18] and -0.85% [17].

We have also calculated the VP correction. Our value for the Uehling part amounts to 0.410%, which agrees well with the previous calculations of this effect. We have found that including the screening into the Uehling potential does not affect this value. As to the Wichmann-Kroll (WK) correction, our calculation employing approximate formulas for the WK potential from Ref. [27] yields -0.004% (cf. [9]). This leads to the 0.406% result for the total VP correction. Therefore, the total binding QED correction amounts to -0.27(3)%.

To get the total $6s$-$7s$ PNC transition amplitude in ^{133}Cs, we combine the value that includes the correlation effects [9], -0.908(5), with the -0.61% Breit correction [9], the -0.27(3)% binding QED correction, the -0.19(6)% neutron skin correction [28], the -0.08% correction due to the renormalization of Q_W from the atomic momentum transfer $q \sim 30$ MeV down to $q = 0$ [17], and the 0.04% contribution from the electron-electron weak interaction [17]. The analysis of accuracy of the atomic structure PNC calculations [7, 9–11] is based on calculations of the hyperfine splitting, decay rates, and energy levels. As it was argued in Ref. [17], QED corrections to these quantities can be neglected on the 0.5% accuracy level. Using the experimental value for $E_{\rm PNC}/\beta$ [4], where β is the vector transition polarizabilty, we obtain for the weak charge of ^{133}Cs:

$$Q_W = -72.57(29)_{\rm exp}(36)_{\rm th} \qquad (16)$$

for $\beta = 26.957(51)a_{\rm B}^3$ [5, 9] and

$$Q_W = -73.09(39)_{\rm exp}(37)_{\rm th} \qquad (17)$$

for $\beta = 27.15(11)a_{\rm B}^3$ [9, 29, 30]. We conclude that the first value deviates from the SM prediction of -73.09(3) [31] by 1.1 σ, while the second one is in perfect agreement with it.

In summary, we have calculated the QED correction to the $6s$-$7s$ PNC transition amplitude in ^{133}Cs and derived the weak charge using two most accurate values of the vector transition polarizability. Further improvement of atomic tests of

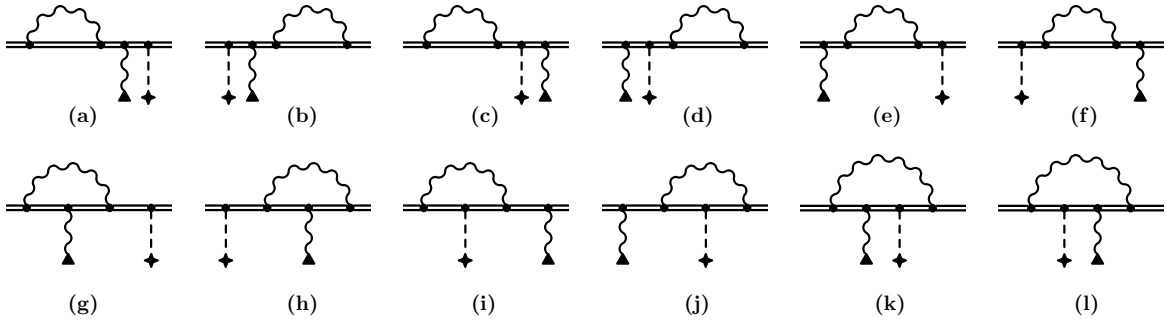

FIG. 1: Feynman diagrams for the SE corrections to the PNC transition amplitude. The wavy line terminated with a triangle indicates the absorbed photon. The dashed line terminated with a cross indicates the electron-nucleus weak interaction.

TABLE II: The SE corrections to the $6s - 7s$ PNC amplitude in ^{133}Cs, in %. The results are presented in both the length (L) and the velocity (V) gauge.

Contr.	L-gauge	V-gauge	Contr.	L-gauge	V-gauge
$\delta E^{\rm a}_{\rm PNC}$	-0.09	-0.11	$\delta E^{\rm h}_{\rm PNC}$	-4.04	-3.40
$\delta E^{\rm b}_{\rm PNC}$	1.31	1.11	$\delta E^{\rm i}_{\rm PNC}$	-4.61	-3.97
$\delta E^{\rm c}_{\rm PNC}$	0.34	0.40	$\delta E^{\rm j}_{\rm PNC}$	1.49	1.73
$\delta E^{\rm d}_{\rm PNC}$	-0.38	-0.32	$\delta E^{\rm k}_{\rm PNC}$	-0.79	-1.03
$\delta E^{\rm e}_{\rm PNC}$	-1.29	-1.53	$\delta E^{\rm l}_{\rm PNC}$	2.05	1.41
$\delta E^{\rm f}_{\rm PNC}$	3.89	3.25	$\delta E^{\rm add}_{\rm PNC}$	0.00	0.10
$\delta E^{\rm g}_{\rm PNC}$	1.33	1.57	$\delta E^{\rm tot}_{\rm PNC}$	-0.79	-0.79
			$\delta E^{\rm bind}_{\rm PNC}$	-0.67	-0.67

the Standard Model can be achieved, from theoretical side, by more accurate calculations of the electron-correlation effects and, from experimental side, by more precise measurements of the PNC amplitude in cesium or other atomic systems.

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