Revisiting Parity Nonconservation in Cesium

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We apply the sum-over-states approach to calculate partial contributions to parity nonconservation (PNC) in cesium [Porsev, Beloy, and Dreviankо, Phys. Rev. Lett. **102**, 181601 (2009)]. We find significant corrections to two nondominating terms coming from the contribution of the core and highly excited states ($n > 9$, the so called tail). When these differences are taken into account the result of Porsev *et al.*, $E_{\rm PNC} = 0.8906(24) \times 10^{-11} i(-Q_W/N)$ changes to 0.8977 (40), coming into good agreement with our previous calculations, 0.8980 (45). The interpretation of the PNC measurements in cesium still indicates reasonable agreement with the standard model (1.5σ); however, it gives new constraints on physics beyond it.

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Introduction.—The search for new physics beyond the standard model using parity nonconservation (PNC) in atoms culminated in 1997 when the Boulder group reported very accurate measurements of the PNC $6s$-$7s$ amplitude in cesium [1]. The experimental uncertainty was only 0.35%. The interpretation of the measurements based on early calculations by the Novosibirsk [2] and Notre Dame [3] groups indicated good agreement with the standard model. However, the declared theoretical accuracy of these early calculations (1%) did not match the accuracy of the measurements. Bennett and Wieman reanalyzed the accuracy of the calculations by comparing calculated observables with new experimental data [4]. They pointed out that many discrepancies between theory and experiment were resolved in favor of theory and suggested that the actual accuracy of the calculations [2,3] was 0.4%. This led to about a 2.3σ deviation of the value of the weak charge of the cesium nucleus from the prediction of the standard model. The discrepancies were resolved when Breit [5,6] and radiative (see, e.g., Ref. [7] and references therein) corrections were included in the calculations. On the other hand, new calculations of the correlations [8,9] did not change the old results of Refs. [2,3] and rather confirmed the suggestion made in Ref. [4] that their accuracy was high. The new value of the weak nuclear charge was about 1σ smaller than the prediction of the standard model, which should be considered as good agreement.

The situation changed when the latest, most sophisticated calculations of the PNC in Cs were reported by Porsev *et al.* [10]. The authors of this work used the sum-over-states approach and applied the coupled cluster with single, double, and valence triple excitations for the leading terms in the sum. They claimed a 0.27% uncertainty for the calculations while their correlated PNC amplitude was about 0.9% smaller than in previous calculations. This led to perfect agreement with the standard model, with central points for the weak nuclear charge extracted from the measurements and predicted by the standard model coinciding exactly: $Q_W(^{133}\mathrm{Cs}) = -73.16(29)_{\rm exp}(20)_{\rm theor}$ and $Q_W^{\rm SM}(^{133}\mathrm{Cs}) = -73.16(3)$ [10]. The smaller value of the correlated PNC amplitude is attributed in Ref. [10] to the role of higher-order correlations.

Although all old and new calculations of the PNC in Cs lead to agreement with the standard model, the results of Ref. [10] have important implications imposing strong constraints on new physics beyond the standard model. Therefore, it is worth studying further the reasons for the difference in the calculations.

The authors of Ref. [10] paid a great deal of attention to the leading terms, performing very sophisticated calculations for them and demonstrating high accuracy by comparing them with available experimental data. The uncertainty for the minor terms was assumed to be 10% based on the spread of the values in different approximations. The sum-over-states approach used in Ref. [10] has an important shortcoming. The calculation of each term in the sum is practically independent of the others and therefore the high accuracy for the leading terms does not guarantee high accuracy for the sum.

In this Letter we use the sum-over-states approach to study possible reasons for the difference between the results of Ref. [10] and previous calculations [2,9]. We assume that the main term was calculated correctly in Ref. [10] and focus our attention on the minor terms such as the contribution of the core states and highly excited (tail) states. We include core polarization and correlation corrections into the core and tail contributions and find a significant difference for both of these terms between our calculations and those reported in Ref. [10]. Our core contribution has a different sign while being similar in value. We have agreement with Ref. [10] for the tail contribution when only core polarization effects are taken into account. However, further inclusion of Bruekner-type correlations increases the PNC amplitude beyond the 10% uncertainty for the tail assumed in Ref. [10].

If the core and tail contributions of Ref. [10] are replaced by the findings of the present work, the resulting PNC amplitude comes into excellent agreement with previous calculations. The application of our calculations to the analysis of the PNC measurements in Cs leads to a value of weak nuclear charge that is about 1.5σ smaller than the value predicted by the standard model. While the PNC amplitude found in this work is practically the same as in Refs. [7,9], the apparent increase in the deviation from the standard model (1σ in Refs. [7,9] when the proper values of the Breit, radiative, and neutron skin corrections are added) is due to smaller uncertainty. This smaller uncertainty is mostly due to the small uncertainty of the main term, which we have taken from Ref. [10] without reanalysis.

The PNC amplitude calculated in this work gives new constraints on physics beyond the standard model.

Calculations.—The PNC amplitude of an electric dipole transition between the $6s$ and $7s$ states of cesium can be written as

$$E_{\mathrm{PNC}} = \sum_n \left[\frac{\langle 6s|H_{\mathrm{PNC}}|np_{1/2}\rangle\langle np_{1/2}|\boldsymbol{d}|7s\rangle}{E_{6s} - E_{np_{1/2}}} + \frac{\langle 6s|\boldsymbol{d}|np_{1/2}\rangle\langle np_{1/2}|H_{\mathrm{PNC}}|7s\rangle}{E_{7s} - E_{np_{1/2}}} \right], \quad (1)$$

where $\boldsymbol{d} = -e\sum_i \boldsymbol{r}_i$ is the electric dipole operator, H_{PNC} is the operator of a P-odd CP-even weak interaction

$$H_{\mathrm{PNC}} = -\frac{G_F}{2\sqrt{2}} Q_W \gamma_5 \rho(\boldsymbol{r}), \quad (2)$$

$G_F \approx 2.2225 \times 10^{-14}$ a.u. is the Fermi constant of the weak interaction, and Q_W is the nuclear weak charge.

Equation (1) is exact if states $6s$, $7s$, $np_{1/2}$ label many-electron physical states of the atom. Then $6s$ is the ground state and the summation goes over the excited states of the opposite parity and the same total angular momentum $J = 1/2$. In practical calculations Eq. (1) is reduced to one with single-electron orbitals and single-electron matrix elements. It looks very similar to Eq. (1) but with a few important differences: (a) All states ($6s$, $7s$, $np_{1/2}$) are now single-electron states obtained with the use of the Hartree-Fock method. (b) Many-electron effects are reduced to the redefinition of the single-electron orbitals and interaction Hamiltonians. For example, the inclusion of the core polarization effect leads to redefinition of the interaction Hamiltonian. For the weak interaction we have $H'_{\mathrm{PNC}} = H_{\mathrm{PNC}} + \delta V_{\mathrm{PNC}}$, where δV_{PNC} is the correction to the self-consistent potential of the atomic core due to the effect of the weak interaction H_{PNC}. For the electric dipole interaction we have a similar expression $\boldsymbol{d}' = \boldsymbol{d} + \delta V_d$. (c) The summation in Eq. (1) now goes over the complete set of single-electron states including states in the core. Extending the summation to the core states corresponds to inclusion of highly excited autoionizing states. (d) The expression of Eq. (1) via single-electron states is approximate. Its accuracy is determined by how the many-body effects are included.

Equation (1) implies the sum-over-states approach which we are going to study in this Letter. As mentioned above, high accuracy for the leading terms does not guarantee high accuracy for the sum. To test the total sum we use an alternative approach which we have used in our previous PNC calculations [2,9]. This approach is based on the solving of differential equations.

The PNC amplitude [Eq. (1)] can be rewritten as

$$E_{\mathrm{PNC}} = \langle \delta\psi_{6s}|\boldsymbol{d}|\psi_{7s}\rangle + \langle \psi_{6s}|\boldsymbol{d}|\delta\psi_{7s}\rangle, \quad (3)$$

where the ψ and $\delta\psi$ are single-electron orbitals and $\delta\psi_a$ is the correction to the wave function ψ_a due to the weak interaction

$$\delta\psi_a = \sum_n \frac{\langle a|H'_{\mathrm{PNC}}|np_{1/2}\rangle}{E_a - E_{np_{1/2}}}\langle np_{1/2}|. \quad (4)$$

It is easy to see that this correction to the wave function satisfies the differential equation

$$(\hat{H}_0 - E_a)\delta\psi_a = -H'_{\mathrm{PNC}}\psi_a. \quad (5)$$

Here ψ_a is the eigenstate of the $\hat{H}_0$ Hamiltonian, which is in our case the relativistic Hartree-Fock Hamiltonian. The left-hand side of Eq. (5) has the form of the relativistic Hartree-Fock equation. However, the energy is fixed and there is also the right-hand side. Solving the differential equation [Eq. (5)] for the $6s$ and $7s$ states of cesium and using Eq. (3) to calculate the PNC amplitude does not require a complete set of single-electron states. To find partial contributions of selected states one needs to impose orthogonality conditions for $\delta\psi_a$ to these states. This method is numerically more stable than the sum-over-states approach. In the present work we use it as an independent test of the calculations. The difference between the two approaches for the partial contributions is less than 0.01% of the the total PNC amplitude.

To perform the summation in Eq. (1) we use the B-spline basis set first presented in Ref. [11]. We use 100 B splines in each partial wave in the cavity of radius 75 a_B. The cavity radius is taken to be the same as in Ref. [10]. Its value is dictated by the need to have the dominating states as close to physical (spectroscopic) states as possible. The most important intermediate states, according to Ref. [10], are the $6p_{1/2}$, $7p_{1/2}$, $8p_{1/2}$, and $9p_{1/2}$ states. The value $R_{\mathrm{max}} = 75a_B$ is large enough for the $9p_{1/2}$ to be a physical state. The number of splines is chosen to be sufficiently large to saturate the summation. It turns out that saturation is achieved at approximately 80 B splines (in Ref. [10] the authors used 40 B splines of a different type).

To compare the tail terms in different calculations, the basis sets must satisfy two conditions. First, the box size and number of splines must be large enough for accurate approximation of all the atomic states entering the main

term so that these states can be associated with real physical states. Second, the basis must be complete. For all basis sets which satisfy both of these conditions the tail does not depend on the basis. We believe that both our basis and that used in Ref. [10] satisfy these conditions.

We include two types of correlations, the core polarization effect and Brueckner type correlations [12]. The core polarization is the effect of the change in the self-consistent Hartree-Fock potential due to an external field. In our case we have two types of external fields, the electric dipole field of the external photon and the weak interaction of atomic electrons with the nucleus. As we mentioned above, the inclusion of the core polarization is reduced to a redefinition of the interaction Hamiltonians (plus the small "electroweak" corrections considered in Refs. [2,9,12]). It is done in the framework of the random phase approximation (RPA).

The Brueckner type correlations describe the correlation interaction of the external electron with the atomic core, which can be reduced to redefinition of the single-electron orbitals, constructing the Brueckner orbitals [12]. For this purpose we calculate the correlation potential $\hat{\Sigma}$ [12,13] and construct linear combinations of B splines which are eigenstates of the $\hat{H}_0 + \hat{\Sigma}$ Hamiltonian. To include correlations in Eq. (5), Brueckner orbitals should be used in the right-hand side and the Hartree-Fock Hamiltonian $\hat{H}_0$ should be replaced by $\hat{H}_0 + \hat{\Sigma}$, where $\hat{\Sigma}$ is the correlation potential used to calculate the Brueckner orbitals.

Results and discussion.—Table I shows the contributions to the PNC amplitude in Cs obtained in different approximations. The correlations have a significant effect on the tail contribution, and there are significant differences in the values of the core and tail contributions between the present work and Ref. [10]. There is also a 1.3% difference for the main term. However, this difference is not important. An accurate treatment of the main term goes beyond the scope of the present Letter; we just take its value from Ref. [10]. If the core and tail terms also have this 1.3% relative uncertainty. that would be more than satisfactory for our purposes; we will see below that the actual uncertainty is larger.

TABLE I. Partial contributions to the $E_{\rm PNC}$ [in $10^{-11}i(-Q_W/N)$ a.u.] for Cs in different approximations.

Approximation	Core	Main	Tail	Total
RPA[a]	0.0026	0.8705	0.0192	0.8923
BO($\hat{\Sigma}^{(2)}$)[b]	0.0015	0.8641	0.0272	0.8928
BO($\lambda\hat{\Sigma}^{(2)}$)[c]	0.0018	0.8709	0.0244	0.8971
BO($\hat{\Sigma}^{(\infty)}$)[d]	0.0018	0.8711	0.0238	0.8967
BO($\lambda\hat{\Sigma}^{(\infty)}$)[e]	0.0018	0.8678	0.0242	0.8938
Ref. [10][f]	−0.0020	0.8823	0.0195	0.8998

[a]Core polarization but no correlations beyond it.
[b]Brueckner orbitals (BO) calculated with the second-order $\hat{\Sigma}$.
[c]BO calculated with rescaled second-order $\hat{\Sigma}$.
[d]BO calculated with the all-order $\hat{\Sigma}$.
[e]BO calculated with rescaled all-order $\hat{\Sigma}$.
[f]DHF for the core term; coupled cluster for the main term.

Core contribution.—Our results for the core are presented in Table II. The result in the Dirac-Hartree-Fock (DHF) approximation is in good agreement with those of Refs. [3,10] (see also Table I), which were calculated in the DHF approximation in both works [14].

Note the strong cancelation between terms with $\delta\psi_{6s}$ and $\delta\psi_{7s}$. This cancelation makes the core contribution very sensitive to the inclusion of the core polarization effect. We include it by solving the RPA equations for both operators ($H_{\rm PNC}$ and $\boldsymbol{d}$). The equations for the electric dipole operator are solved at $\omega = 0.0844$ a.u., which is the experimental energy difference between the $6s$ and $7s$ states of Cs.

The last line of Table II presents the effect of using Brueckner orbitals for the core contribution. The use of Brueckner orbitals in the core can be justified by the condition that the core and valence states must be orthogonal to each other, and using the same $\hat{\Sigma}$ operator in both cases is a good way to achieve this. The difference in the core contribution using the RPA and Brueckner orbitals is relatively small (see Table I). We use this difference as an estimate of the uncertainty of the core contribution.

Due to the high sensitivity of the core contribution to different corrections we found it useful to perform one more test. We ran our code for the PNC in Ra^+ and found excellent agreement with Ref. [15] for the core contribution in the RPA.

The final difference between the present work and Ref. [10] for the core contribution is 0.0038 in units of Table II. This difference is mostly due to the core polarization effect.

Tail contribution.—The third row of Table I shows the partial contributions to the tail component of the PNC amplitude calculated in different approximations. To include correlations we use four different sets of Brueckner orbitals obtained with the use of two different correlation-correction operators $\hat{\Sigma}$: the second-order operator $\hat{\Sigma}^{(2)}$ [12]; and the all-order operator $\hat{\Sigma}^{(\infty)}$ [13]. The rescaling of $\hat{\Sigma}$ is done to fit the energies of the lowest

TABLE II. Contributions of the core states $np_{1/2}$ to the $E_{\rm PNC}$ [in $10^{-11}i(-Q_W/N)$ a.u.] for Cs in different approximations.

	$\langle\delta\psi_{6s}\|\boldsymbol{d}\|\psi_{7s}\rangle$	$\langle\psi_{6s}\|\boldsymbol{d}\|\delta\psi_{7s}\rangle$	Sum
DHF	0.02471	−0.02645	−0.00174
RPA[a]	0.05991	−0.05821	0.00170
RPA[b]	0.06043	−0.05784	0.00259
BO + RPA[b]	0.07231	−0.07049	0.00182

[a]RPA equations solved at Hartree-Fock frequency.
[b]RPA equations solved at experimental frequency, $\omega = 0.0844$ a.u.

TABLE III. Correlated PNC amplitude in Cs [in $10^{-11}i(-Q_W/N)$ a.u.] in different calculations. Breit, QED, and neutron skin corrections are not included.

Value	Source and method
0.908 (9)	CP + PTSCI, Ref. [2]
0.909 (9)	CC SD, Ref. [3]
0.905 (9)	MBPT with fitting, Ref. [8]
0.9078 (45)	CP + PTSCI, Ref. [9]
0.8998 (24)	CC SDvT, Ref. [10]
0.9079 (40)	This work

valence states. Rescaling usually improves the wave functions and therefore the matrix elements.

Inclusion of the correlations leads to a significant increase in the values of the tail contribution (see Table I). For our final number we take our most complete calculation, using the all-order $\hat{\Sigma}$ operator, while the spread of values in the various Brueckner approximations gives a reliable estimate of the uncertainty in our methods.

The result of Ref. [10] for the tail (0.0195, see Table I) was obtained using a blend of many-body approximations including a simplified coupled-cluster method which only includes single and double excitations [14]. Note that our all-order correlation potential $\hat{\Sigma}$ includes multiple excitations [13]. The result of Ref. [10] for the tail is close to our result in the RPA but significantly smaller than our correlated value.

Summary.—Table III presents the results of the most accurate calculations of the correlated [without Breit, quantum electrodynamic (QED), and neutron skin correction] PNC amplitude in Cs. The abbreviation CP + PTSCI stands for correlation potential [12] combined with the perturbation theory in screened Coulomb interaction, CC SD stands for coupled cluster with single and double excitations, CC SDvT means coupled cluster with single, double, and valence triple excitations. All numbers, apart from those of Ref. [10] are in very good agreement with each other. But if the result of Ref. [10] is corrected as shown in Table I, it comes to very good agreement with the other calculations as well (last line of Table III).

We summarize the results in Table IV. We take the main term from Ref. [10] assuming that its value and uncertainty were calculated correctly. The core and tail contributions come from the present work. Then we add all other significant contributions to the PNC amplitude in cesium which can be found in the literature. The final value for the PNC amplitude is

$$E_{\mathrm{PNC}} = 0.8977(40) \times 10^{-11} i(-Q_W/N), \tag{6}$$

which is in excellent agreement with our previous calculations, $E_{\mathrm{PNC}} = 0.8980(45)$ [7,9]. The experimental value for the PNC amplitude is [1]

$$E_{\mathrm{PNC}}/\beta = 1.5935(56)\ \mathrm{mV/cm}. \tag{7}$$

TABLE IV. All significant contributions to the E_{PNC} [in $10^{-11}i(-Q_W/N)$ a.u.] for Cs.

Contribution	Value	Source
Core ($n < 6$)	0.0018 (8)	This work
Main ($n = 6$–9)	0.8823 (17)	Ref. [10]
Tail ($n > 9$)	0.0238 (35)	This work
Subtotal	0.9079 (40)	This work
Breit	−0.0055 (1)	Refs. [5,6]
QED	−0.0029 (3)	Ref. [7]
Neutron skin	−0.0018 (5)	Ref. [5]
Total	0.8977 (40)	This work

The most accurate value for the vector transition probability β comes from the analysis [16] of the Bennett and Wieman measurements [17]

$$\beta = 26.957(51)a_B^3. \tag{8}$$

Comparing Eqs. (6)–(8), leads to

$$Q_W(^{133}\mathrm{Cs}) = -72.58(29)_{\mathrm{expt}}(32)_{\mathrm{theory}}. \tag{9}$$

This value is in a reasonable agreement with the prediction of the standard model, $Q_W^{\mathrm{SM}} = -73.23(2)$ [18]. If we add theoretical and experimental errors in Eq. (9) in quadrature, the Cs PNC result deviates from the standard model value by 1.5σ:

$$Q_W - Q_M^{\mathrm{SM}} \equiv \delta Q_W = 0.65(43). \tag{10}$$

For small deviations from the standard model values we may relate this to the deviation in $\sin^2\theta_W$ using the simple relationship $\delta Q_W \approx -4Z\delta(\sin^2\theta_W)$ which gives

$$\sin^2\theta_W = 0.2356(20). \tag{11}$$

This is also 1.5σ off the standard model value 0.2386 (1) [18] at near zero momentum transfer.

The new physics originating through vacuum polarization to gauge boson propagators is described by weak isospin conserving S and isospin breaking T parameters [19]

$$Q_W - Q_M^{\mathrm{SM}} = -0.800S - 0.007T. \tag{12}$$

At the 1σ level Eq. (10) leads to $S = -0.81(54)$.

Finally, a positive ΔQ_W could also be indicative of an extra Z boson in the weak interaction [20]

$$Q_W - Q_M^{\mathrm{SM}} \approx 0.4(2N + Z)(M_W/M_{Z_\chi})^2. \tag{13}$$

Using Eq. (10) leads to $M_{Z_\chi} > 710\ \mathrm{GeV}/c^2$.

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