We apply the sum-over-states approach to calculate partial contributions to the parity non-conservation (PNC) in cesium [Porsev et al, Phys. Rev. D 82, 036008 (2010)]. We have found significant corrections to two non-dominating 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, \( E_{\text{PNC}} = 0.8906 \times 10^{-11} \) changes to \( 0.8977 \), coming into good agreement with our previous calculations, \( 0.8980 \). The interpretation of the PNC measurements in cesium still indicates reasonable agreement with the standard model (1.5\( \sigma \)), however gives new constraints on physics beyond it.

PACS numbers: 11.30.Er, 31.15.A-

INTRODUCTION

The search for new physics beyond standard model using parity non-conservation (PNC) in atoms culminated in 1997 when Boulder group reported very accurate measurements of the PNC 6s - 7s amplitude in cesium [1]. The experimental uncertainty was only 0.35\%. Interpretation of the measurements based on early calculations by Novosibirsk [2] and Notre Dame [3] groups indicated good agreement with the standard model. However, the declared theoretical accuracy of these early calculations (1\%) didn’t match the accuracy of the measurements. Bennett and Wieman re-analyzed 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 actual accuracy of the calculations [2,3] was 0.4\%. This lead to about 2.3\( \sigma \) deviation of the value of the weak charge of the cesium nucleus from the prediction of the standard model. The discrepancy were resolved when Breit [5,6] and radiative (see, e.g [7] and references therein) corrections were included into calculations. On the other hand, new calculations of the correlations [8,9] didn’t change the old results of [2,3] and rather confirmed the suggestion made in [2] that their accuracy was high. The new value of the weak nuclear charge was about 1\( \sigma \) 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 0.27\% uncertainty of 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: \( Q_W^{(133)} = -73.16(29) \) and \( Q_W^{(133)} = -73.16(30) \). The smaller value of the correlated PNC amplitude is attributed in [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 [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 [10] paid great deal of attention to the leading terms, performing very sophisticated calculations for them and demonstrating high accuracy by comparing 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 [10] has an important shortcoming. Calculation of each term in the sum is practically independent of others and therefore the high accuracy for the leading terms does not guarantee high accuracy for the sum.

In this paper we use the sum-over-states approach to study possible reasons for the difference between the results of [10] and previous calculations [2,3]. We assume that the main term was calculated correctly in [10] and focus our attention on the minor terms such us 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 significant difference for both these terms between our calculations and those reported in [10]. Our core contribution has different sign while being similar in value. We have agreement with [10] for the tail contribution when only core polarization effects are taken into account. However, further inclusion of Brueckner-type correlations increase the PNC amplitude beyond the 10\% uncertainty for the tail assumed in [10].

If core and tail contributions of [10] are replaced by
the findings of 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 1.5 $\sigma$ smaller than the value predicted by the standard model. While the PNC amplitude found in this work is practically the same as in Ref. [7, 9], the apparent increase in deviation from the standard model (1 $\sigma$ in Ref. [7, 9] when proper values of the Breit, radiative and neutron skin corrections are added) is due to smaller uncertainty. This smaller uncertainty is mostly due to small uncertainty of the main term which we have taken from Ref. [10] without re-analysis.

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

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

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

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

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

Expression (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 summation goes over excited states of the opposite parity and the same total angular momentum $J = 1/2$. In practical calculations equation (1) is reduced to one with single-electron orbitals and single-electron matrix elements. It looks very similar to (1) but with a few important differences. (a) All states ($6s$, $7s$ and $np_{1/2}$) are now single-electron states obtained with the use of the Hartree-Fock method. (b) Many-electron effects are reduced to 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 $H'_{\text{PNC}} = H_{\text{PNC}} + \delta V_{\text{PNC}}$, where $\delta V_{\text{PNC}}$ is the correction to the self-consistent potential of the atomic core due to the effect of weak interaction $H_{\text{PNC}}$. For the electric dipole interaction we have similar expression $d' = d + \delta V_d$. (c) Summation in (1) now goes over the complete set of single-electron states including states in the core. Extending summation to the core states corresponds to inclusion of highly excited autoionizing states. (d) The expression (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 paper. 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 (1) can be rewritten as

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

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

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

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

$$ (H_0 - E_a) \delta \psi_a = -H'_{\text{PNC}} \psi_a. \quad (5) $$

Here $\psi_a$ is the eigenstate of the $H_0$ Hamiltonian, which is in our case the relativistic Hartree-Fock (RHF) Hamiltonian. The equations (3) have a form of the RHF equations with the right-hand side. Solving differential equation (5) for the $6s$ and $7s$ states of cesium and using (4) to calculate the PNC amplitude does not require a complete set of single-electron states. It is usually numerically more accurate than the use of the sum-over-states approach. In present work we use it as an independent test of the calculations.

To perform the summation in (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 be as close to physical (spectroscopic) states as possible. The most important intermediate states, according to [10], are the $6p_{1/2}$, $7p_{1/2}$, $8p_{1/2}$, and $9p_{1/2}$ states. The value $R_{\text{max}} = 75 a_B$ is large enough for the $9p_{1/2}$ to be 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 [11] 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 the all atomic states entering main term so that these states can be associated with real physical states. Second, the basis must be complete. For all basis
The total PNC amplitude in the this approximation obtained via solving equations (SE) \((5)\) and then using for-

\[ R_{\text{PA}} \text{ approximation obtained with the direct summation (DS)} \]

\[ \text{total PNC amplitude in the this approximation obtained with the direct summation (DS)} \]

\[ \text{considered in detail below. Here we start our discussion with some general remarks. The total PNC amplitude in the RPA approximation obtained with the direct summation (DS) is} \]

\[ E_{\text{RPA}}(\text{DS}) = 0.89235 \times 10^{-11} i(-Q_W/N). \]

The total PNC amplitude in the this approximation obtained via solving equations (SE) \([3]\) and then using for-

\[ \text{results and discussion} \]

\[ \text{Table I shows contributions to the PNC amplitude in Cs obtained in different approximations within the sumover-states approach. Partial contributions will be considered in detail below. Here we start our discussion with some general remarks. The total PNC amplitude in the RPA approximation obtained with the direct summation (DS) is} \]

\[ E_{\text{RPA}}(\text{DS}) = 0.89235 \times 10^{-11} i(-Q_W/N). \]

\[ \text{Note the excellent agreement between these two numbers. Since both methods of calculation share very little in common, it is safe to assume that numerical error is negligible in both cases and the number truly represents the PNC amplitude in the RPA approximation. This implies high quality of the basis used in present work and its suitability to study partial contributions.} \]

\[ \text{Table II shows significant effect of correlations on the tail contribution and significant difference in the values of core and tail contributions between present work and} \]

\[ \text{Note the excellent agreement between these two numbers. Since both methods of calculation share very little in common, it is safe to assume that numerical error is negligible in both cases and the number truly represents the PNC amplitude in the RPA approximation. This implies high quality of the basis used in present work and its suitability to study partial contributions.} \]

\[ \text{Core contribution} \]

\[ \text{Calculations in the present work are done in two different ways. One uses the sum-over-states approach and limits the summation in} \]

\[ \text{Note the excellent agreement between these two numbers. Since both methods of calculation share very little in common, it is safe to assume that numerical error is negligible in both cases and the number truly represents the PNC amplitude in the RPA approximation. This implies high quality of the basis used in present work and its suitability to study partial contributions.} \]

\[ \text{Core contribution} \]

\[ \text{Calculations in the present work are done in two different ways. One uses the sum-over-states approach and limits the summation in} \]

\[ \text{Note the excellent agreement between these two numbers. Since both methods of calculation share very little in common, it is safe to assume that numerical error is negligible in both cases and the number truly represents the PNC amplitude in the RPA approximation. This implies high quality of the basis used in present work and its suitability to study partial contributions.} \]
The electric dipole operator are solved at both operators (\(H_{\text{PNC}}\) and \(d\)). 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 I presents the effect of using Brueckner orbitals for the core contribution. The use of the Brueckner orbitals in the core can be justified by the condition that core and valence states must be orthogonal to each other and using the same \(\Sigma\) operator in both cases is a good way to achieve this. The difference in the core contribution using RPA and Brueckner orbitals is relatively small (see Table I). We use this difference as an estimate of the uncertainty of the core contribution.

The final difference between the present work and [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 II shows 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 \(\Sigma\): the second-order operator \(\Sigma^{(2)}\) [12]; and the all-order operator \(\Sigma^{(\infty)}\) [13]. Rescaling of \(\Sigma\) is done to fit the energies of the lowest valence states. Rescaling usually improves the wave functions and therefore the matrix elements.

Inclusion of the correlations leads to 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 \(\Sigma\) operator, while the spread of values in the various Brueckner approximations gives a reliable estimate of the uncertainty in our methods.

The result of [10] for the tail (0.0195, see Table II) was obtained using a blend of many-body approximations including a simplified coupled-cluster method which only includes single and double excitations [15]. The result is close to our result in the RPA approximation but significantly smaller than our correlated value.

### Summary

Table III presents the results of the most accurate calculations of the correlated (without Breit, quantum electrodynam (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 [10] is corrected as shown in Table I it comes to very good agreement with 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

\[
E_{\text{PNC}} = 0.8977 (40) \times 10^{-11} i(\beta Q_{W}/N),
\]

which is in excellent agreement with our previous calculations, \(E_{\text{PNC}} = 0.8980 (45)\) [7, 9]. The experimental value for the PNC amplitude is [17]

\[
E_{\text{PNC}}/\beta = 1.5935 (56) \text{ mV/cm}.
\]

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

\[
\beta = 26.957 (51) a_B^3.
\]

Comparing [15], [17] and [8] leads to

\[
Q_W^{(133\text{Cs})} = -72.58 (29)_{\text{expt}} (32)_{\text{theory}}.
\]

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

$$Q_W - Q_{SM} = 0.65 \text{(43).}$$  \hspace{1cm} (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

$$\sin^2 \theta_W = 0.2356 \text{(20).}$$  \hspace{1cm} (11)

This is also $1.5 \sigma$ off the standard model value $0.2386 \text{ (1) [18]}$ at near zero momentum transfer.

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

$$Q_W - Q_{SM} = -0.800 S - 0.007 T.$$  \hspace{1cm} (12)

At the $1\sigma$ level $[10]$ leads to $S = -0.81 \text{ (54).}$

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

$$Q_W - Q_{SM} \approx 0.4(2N + Z)(M_W/M_Z)^2.$$  \hspace{1cm} (13)

Using $[10]$ leads to $M_Z > 710 \text{ GeV/c}^2$.

The authors are grateful to A. Derevianko for useful discussions. The work was supported in part by the Australian Research Council.

[1] C. S. Wood, S. C. Bennett, D. Cho, B. P. Masterson, J. L. Roberst, C. E. Tanner, and C. E. Wieman, Science 275, 1759 (1997).