Breit Interaction and Parity Non-conservation in Many-Electron Atoms

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We present accurate ab initio non-perturbative calculations of the Breit correction to the parity non-conserving (PNC) amplitudes of the 6s−7s and 6s−5d3/2 transitions in Cs, 7s−8s and 7s−6d3/2 transitions in Fr, 6s−5d3/2 transition in Ba+, 7s−6d3/2 transition in Ra+, and 6p1/2−6p3/2 transition in Tl. The results for the 6s−7s transition in Cs and 7s−8s transition in Fr are in good agreement with other calculations while calculations for other atoms/ transitions are presented for the first time. We demonstrate that higher-orders many-body corrections to the Breit interaction are especially important for the s − d PNC amplitudes. We confirm good agreement of the PNC measurements for cesium and thallium with the standard model.

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I. INTRODUCTION

Study of the parity non-conservation (PNC) in atoms have reached the accuracy where small corrections like Breit interaction and radiative corrections play significant role (see, e.g. review †). For example, experimental accuracy for the PNC in cesium is 0.35% ‡. Interpretation of this result using earlier atomic calculations § § lead to apparent disagreement with the standard model ‡. This disagreement had been resolved when Breit † † and radiative ‡ ‡ corrections were included into analysis.

In present paper we revisit Breit corrections to the PNC amplitudes in many-electron atoms. Previous calculations were focused on the 6s−7s PNC amplitude in Cs § §, while some also considered very similar (in terms of electron structure) 7s−8s PNC amplitude in Fr † † †. The results are considered to be in reasonable agreement with each other in spite of some difference in the final values given by different calculations (up to ~30%). This is because Breit correction to the PNC amplitude in cesium was small (~0.6%) and relatively rough estimations were sufficient for the sake of the interpretation of the experimental measurements.

However, if we need to calculate Breit corrections to PNC in atoms heavier than cesium or, in general, if we want to have a reliable method to study the effect of Breit interaction in heavy many-electron atoms the important question to ask is what kind of approach should be used to do this? The answer is evident from the analysis of the calculations of Breit contributions by means of many-body perturbation theory (MBPT). The analysis reveals very poor convergence of the MBPT with respect to the number of residual Coulomb interactions included into the higher-order terms. This means that some all-order technique is needed to sum up important chains of higher-order terms to all orders. The natural choice is to present inter-electron interaction as a sum of Coulomb and Breit terms and to treat both terms the same way.

We have developed such approach in our previous work †† and applied it to the analysis of the PNC in cesium. Breit and Coulomb interaction were equally treated on the self-consistent field level (Hartree-Fock and random-phase approximation calculations). However, inclusion of the Breit interaction into calculation of the correlations was not comprehensive. In that work we included correlations by calculating the correlation potential ˆΣ thus achieving equal and comprehensive treatment of Coulomb and Breit interactions on levels up to second order. The method developed in present work is important for many-electron atoms. The results for Tl, Ba+, Ra+ as well as for the s − d transitions for Cs and Fr are presented for the first time.

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II. THEORY

We use the following form of the Breit operator (atomic units are used throughout the paper)

$$\hat{H}^B = \frac{\alpha_1 \cdot \alpha_2 + (\alpha_1 \cdot \hat{n})(\alpha_2 \cdot \hat{n})}{2r}$$  \hspace{1cm} (1)

Here $\mathbf{r} = \hat{n}\mathbf{r}$, $r$ is distance between electrons and $\alpha_i$ is $\alpha$-matrix of the corresponding electron. This is a low frequency limit of the relativistic correction to the Coulomb interaction between electrons. It contains magnetic interaction and retardation.

Similar to Coulomb interaction, Breit interaction creates self-consistent Breit potential

$$\hat{V}^B \psi_n(r) = \sum_n \left( \int \psi_n^\dagger \hat{H}^B \psi_n d^3r' \psi(r) - \int \psi_n^\dagger \hat{H}^B \psi d^3r' \psi_n(r) \right).$$  \hspace{1cm} (2)

Here summation goes over all core states. In the case of closed-shell atoms (like alkali atoms in the $V^{N-1}$ approximation) direct term in Breit potential vanishes (first term in (2)) and only second, exchange, term remains.

Hartree-Fock Hamiltonian has the form

$$\hat{H}_0 = c \alpha \mathbf{p} + (\beta - 1)mc^2 - \frac{Ze^2}{r} + \hat{V},$$  \hspace{1cm} (3)

where $\hat{V}$ is the self-consistent potential created by electrons from the core. To achieve comprehensive treatment of the Breit interaction potential $\hat{V}$ should be presented as a sum of Coulomb and Breit terms

$$\hat{V} = \hat{V}^C + \hat{V}^B.$$  \hspace{1cm} (4)

Note that we write for simplicity nuclear potential in (4) as for point-like nucleus. However, our actual potential takes into account finite nuclear size.

To do PNC calculations one needs to take into account dipole interaction of an atom with external photon as well as weak interaction of atomic electrons with the nucleus. We use the time-dependent Hartree-Fock method (TDHF) to do this. This method is equivalent to well-known random-phase approximation (RPA).

For every electron in the atom, single electron wave function is presented in the form

$$\tilde{\psi}_n = \psi_n + \delta \psi_n + X_n e^{-i\omega t} + Y_n e^{i\omega t} + \delta X_n e^{-i\omega t} + \delta Y_n e^{i\omega t},$$  \hspace{1cm} (5)

where index $n$ numerates single-electron states, $\psi_n$ is unperturbed wave function for the state $n$ which is an eigenstate of the Hartree-Fock Hamiltonian. $\delta \psi_n$ is correction to $\psi_n$ due to weak interaction with the nucleus, $X_n$ and $Y_n$ are corrections due to electric field of external photon of frequency $\omega$, $\delta X_n$ and $\delta Y_n$ are corrections due to simultaneous action of the weak interaction and dipole interaction with external photon.

Corrections $\delta \psi_n$, $X_n$, $Y_n$, $\delta X_n$, $\delta Y_n$ to all atomic states found by self-consistent iteration of the TDHF equations:

$$\left( \hat{H}_0 - \epsilon_n \right) \delta \psi_n = -\left( \hat{H}_W + \delta \hat{V}_W \right) \psi_n,$$  \hspace{1cm} (6)

$$\left( \hat{H}_0 - \epsilon_n - \omega \right) X_n = -\left( \hat{H}_{E1} + \delta \hat{V}_{E1} \right) \psi_n,$$  \hspace{1cm} (7)

$$\left( \hat{H}_0 - \epsilon_n + \omega \right) Y_n = -\left( \hat{H}_{E1} + \delta \hat{V}_{E1} \right) \psi_n,$$  \hspace{1cm} (8)

$$\hat{H}_0 - \epsilon_n = X_n - \hat{V} E_{1W} \psi_n.$$  \hspace{1cm} (9)

Here $\delta \hat{V}$ is correction to the self-consistent Hartree-Fock potential $\hat{V}$ due to external field (weak ($W$), dipole electric ($E1$) or both ($E1W$)). Equations (6,7,8) are first solved self-consistently for states in the core. Then corrections to valence states are calculated in the field of frozen core.

PNC amplitude for the transition between valence states $a$ and $b$ in the TDHF approximation is

$$E_{PNC}^{TDHF} = \langle \psi_b | \hat{H}_{E1} + \delta \hat{V}_{E1} | \delta \psi_a \rangle + \langle \psi_b | \hat{H}_W + \delta \hat{V}_W | X_a \rangle + \langle \psi_b | \delta \hat{V}_{E1W} | Y_a \rangle.$$  \hspace{1cm} (10)

Breit interaction is included by using expression (4) for the self-consistent potential on all stages of the calculations. In other words, Hartree-Fock amplitude in the left-hand side of equations (6,7,8) is the sum of Coulomb and Breit terms. Correction to the potential $\delta \hat{V}$ in the right-hand side of equations (6,7,8,9) is also the sum of Coulomb and Breit terms:

$$\delta \hat{V} = \delta \hat{V}^C + \delta \hat{V}^B.$$  \hspace{1cm} (11)

Expression (11) does not take into account correlations. To include correlations we introduce correlation potential $\Sigma$. It is defined in such a way that its average value over particular valence state $a$ is the correlation correction to the energy of this state (see, e.g. [12] for details):

$$\Delta \epsilon_a = \langle a | \hat{\Sigma} | a \rangle.$$  \hspace{1cm} (12)

$\hat{\Sigma}$ is a non-local operator which depends on energy and parameter $\kappa$ which defines the angular part of wave function $\psi_a$: $\kappa_a = (-1)^{l_a + j_a + 1/2}(2j_a + 1/2)$, where $l_a$ is angular momentum and $j_a$ is total momentum of state $a$.

In linear in $\hat{\Sigma}$ approximation, correlation correction to the PNC amplitude is

$$\Delta E_{PNC} = \langle \psi_b | \hat{\Sigma}_{\kappa_a} (\epsilon_b) | \delta X_a \rangle + \langle \delta \psi_b | \hat{\Sigma}_{-\kappa_a} (\epsilon_b) | X_a \rangle + \langle \delta \psi_b | \hat{\Sigma}_{\kappa_a} (\epsilon_b) | Y_a \rangle + \langle \psi_b | \hat{\Sigma}_{-\kappa_a} (\epsilon_b) | \delta \psi_a \rangle.$$  \hspace{1cm} (13)
In the most precise calculations of the PNC in cesium \(3, 17\), operator \(\Sigma\) was calculated in all orders in Coulomb interaction. For the purpose of the present work we can restrict ourself with the lowest, second-order expression for \(\Sigma\). Corresponding Brueckner-Goldstone diagrams are presented on Fig. 1. Breit interaction is included in calculation of \(\Sigma\) in two ways. First, a complete set of single-electron states used to calculate \(\Sigma\) was obtained with the use of the Hartree-Fock Hamiltonian \(15\) with Breit potential included as in eq. (1). Second, inter-electron interaction in \(\Sigma\) is already approximate. Non-linear terms can be easily eliminated by a rescaling procedure. In this procedure inter-electron interaction is considered as a sum \((\hat{H}^B)^2, (\hat{H}^B)^3, \ldots\) in which Breit interaction \(\hat{H}^B\) is multiplied by a scaling parameter \(\lambda\). By running programs for different values of \(\lambda\) a range of values is found for which final answer is linear function of \(\lambda\). Then the answer is interpolated to \(\lambda = 1\). It turns out, however, that as a rule \(\lambda = 1\) is already in linear regime.

Finally we note that non-perturbative treatment of Breit interaction leads to inclusion of higher-order in Breit operator terms, terms proportional to \((\hat{H}^B)^2, (\hat{H}^B)^3, \ldots\) with \(\hat{H}^B\) given by (11). Inclusion of these terms cannot be justified since expression (11) is already approximate. Non-linear terms can be easily eliminated by a rescaling procedure. In this procedure inter-electron interaction is considered as a sum \((\hat{H}^B)^2, (\hat{H}^B)^3, \ldots\) in which Breit interaction \(\hat{H}^B\) is multiplied by a scaling parameter \(\lambda\). By running programs for different values of \(\lambda\) a range of values is found for which final answer is linear function of \(\lambda\). Then the answer is interpolated to \(\lambda = 1\). It turns out, however, that as a rule \(\lambda = 1\) is already in linear regime.

### III. RESULTS AND DISCUSSION

Table (II) presents results of calculations of the Breit correction to the PNC amplitudes in Cs, Ba, Tl, Fr and Ra. This is the full list of atoms with one external electron above closed shells for which PNC measurement has been carried out or planned. Comparison with other calculations for the \(6s - 7s\) transition in Cs and \(7s - 8s\) transition in Fr are presented in Table (VII). The results for other atoms and for the \(s - d\) transitions in Cs and Fr are presented for the first time.

Note that for all PNC amplitudes presented in Table (II) the effect of correlations on Breit correction is small in \(\Sigma(2)\) approximation. It becomes significant for some \(s-d\) amplitudes only in Brueckner approximation. This is because the correlation corrections in \(d\)-wave are large and significantly change density of the valence electron inside electron core. Therefore, we should perform calculations using Brueckner orbitals which include \(\Sigma\) to all orders. The linear in \(\Sigma\) expressions (14), (15) do not provide satisfactory accuracy.

As one can see from Table (II) the behavior of \(s-s\) and \(s-d\) PNC amplitudes is very different. Let us discuss them separately. It is convenient to use the sum-over-states expression for the E1 PNC amplitude for the discussion:

\[
E_{1PN C}(ab) = \sum_n \frac{\langle b|\hat{D}|a\rangle \langle a|\hat{W}|n\rangle}{E_a - E_n} + \sum_n \frac{\langle b|\hat{W}|n\rangle \langle n|\hat{D}|a\rangle}{E_b - E_n},
\]
where $\hat{D}$ is electric-dipole operator and $\hat{W}$ is weak interaction operator. In the RPA approximation, $\hat{D} = H_{E1} + \delta V_{E1}$ and $\hat{W} = H_{W} + \delta V_{W}$. Equation (16) is an accurate expression for the E1 PNC amplitude if all states $|a\rangle, |b\rangle, |n\rangle$ are exact many-electron states of the whole atom. However, for our discussion we will consider only states which differ from the ground state by excitation of the single valence electron. This is reasonably good approximation for alkali atoms and it is sufficient for the discussion. In this case matrix elements in (16) are reduced to single-electron matrix elements and we will refer to this expression as sum over single-electron states.

As one can see from Table I, Breit contribution to the correlation correction to the $s - s$ PNC amplitudes is small. This can be explained the following way. Breit and weak interactions are both short-range operators. They have significant value in the vicinity of nucleus where all single-electron wave functions are similar and differ by normalization only. Indeed, Dirac equation for all low states is the same on short distances since energy can be neglected compared to the nuclear potential. On the other hand, higher states with large energies do not contribute to the sum (16) due to large energy denominator. Therefore, relative value of Breit correction to all weak matrix elements in (16) is the same and can be presented as a common factor outside of the summation. The effect of correlations on short distances can also be reduced to change of normalization of the wave function. Therefore, relative Breit correction should remain the same.

This way of argument was used in calculating radiative corrections to the PNC amplitude in cesium [9, 10, 11, 12]. Moreover, it was assumed in [10] that to find radiative correction it is sufficient to consider only corrections to the weak matrix elements. Radiative corrections to E1 transition amplitudes and energies were not considered because it was believed that corresponding contritions to the PNC amplitude are small and can be neglected. It was demonstrated in [12] that radiative corrections to the PNC amplitude in cesium due to change of energy denominators and change of E1 transition amplitudes (see, eq. (16)) are not so small when taken separately. But they cancel each other almost exactly when taken together.

It is interesting to note that very similar situation takes place for the Breit correction. As it was first demonstrated by Derevianko [8, 14] and then confirmed by Dzuba et al. [7], the effects of Breit interaction on the PNC amplitude in cesium due to change of energy de-

| Atom | Z | Transition | Approximation | Coulomb only | Coulomb + Breit | $\Delta$ | $\Delta/EPNC(\%)$ |
|------|---|------------|---------------|--------------|---------------|--------|----------------|
| Cs   | 55| 6s$_{1/2} - 7s_{1/2}$ | TDHF$^a$ | 0.8903 | 0.8849 | -0.0054 | -0.61 |
|      |   |            | $\hat{\Sigma}^{(2)}_{b}$ | 0.9316 | 0.9258 | -0.0058 | -0.62 |
|      |   |            | Br$^c$ | 0.9001 | 0.8945 | -0.0056 | -0.62 |
|      |   | 6s$_{1/2} - 5d_{5/2}$ | TDHF$^a$ | 3.1177 | 3.1012 | -0.0165 | -0.53 |
|      |   |            | $\hat{\Sigma}^{(2)}_{b}$ | 3.5371 | 3.5195 | -0.0176 | -0.50 |
|      |   |            | Br$^c$ | 3.7277 | 3.7165 | -0.0112 | -0.30 |
| Ba$^+$ | 56| 6s$_{1/2} - 5d_{5/2}$ | TDHF$^a$ | 2.1678 | 2.1513 | -0.0165 | -0.76 |
|      |   |            | $\hat{\Sigma}^{(2)}_{b}$ | 2.2091 | 2.1915 | -0.0176 | -0.80 |
|      |   |            | Br$^c$ | 2.1826 | 2.1653 | -0.0173 | -0.79 |
| Tl   | 81| 6p$_{1/2} - 6p_{3/2}$ | TDHF$^a$ | 30.384 | 30.105 | -0.279 | -0.92 |
|      |   |            | $\hat{\Sigma}^{(2)}_{b}$ | 23.157 | 22.941 | -0.216 | -0.93 |
|      |   |            | Br$^c$ | 24.270 | 24.046 | -0.224 | -0.92 |
| Fr   | 87| 7s$_{1/2} - 8s_{1/2}$ | TDHF$^a$ | 16.043 | 15.891 | -0.152 | -0.95 |
|      |   |            | $\hat{\Sigma}^{(2)}_{b}$ | 15.884 | 15.729 | -0.155 | -0.98 |
|      |   |            | Br$^c$ | 15.229 | 15.079 | -0.150 | -0.98 |
| Ra$^+$ | 88| 7s$_{1/2} - 6d_{5/2}$ | TDHF$^a$ | 52.118 | 51.678 | -0.440 | -0.84 |
|      |   |            | $\hat{\Sigma}^{(2)}_{b}$ | 55.568 | 55.103 | -0.465 | -0.84 |
|      |   |            | Br$^c$ | 56.437 | 56.090 | -0.347 | -0.61 |

$^a$TDHF: time-dependent Hartree-Fock, Eq. [9]
$^b$\(\hat{\Sigma}^{(2)}\): second-order correlations are included, Eq. [10]
$^c$Br: Brueckner orbitals, Eq. [16]
TABLE II: Relative Breit correction to weak matrix elements of Cs, Ba\(^+\), Tl, Fr, and Ra\(^+\).

| Atom/Ion | s – p | p – d |
|----------|-------|-------|
| Cs       | -0.58%| -0.03%|
| Ba\(^+\) | -0.65%| -0.29%|
| Tl       | -1.17%| -0.81%|
| Fr       | -0.98%| +1.60%|
| Ra\(^+\) | -1.03%| +0.85%|

Arguments in favor of the small role of correlations presented above for the \(s – s\) PNC amplitudes were based on the fact that both Breit and weak interactions are localized on short distances. While it is true for the “bare” operator of the weak interaction, it is not exactly true when many-body effects are also included. The effective operator of the weak interaction can be presented in the form

\[
\hat{H}_{\text{eff}} = \hat{H}_W + \delta \hat{V}_W, \tag{17}
\]

where first term is proportional to nuclear density and is zero everywhere outside the nucleus. Second term is due to change in self-consistent Hartree-Fock potential because of the effect of weak interaction. It describes the so-called core polarization effect and its radius is roughly equal to the radius of atomic core. For the \(s – p\) matrix elements core polarization is just small correction to the leading first term. Therefore all considerations based on assumption that weak interaction is localized on short distances are still approximately valid.

For the \(p – d\) weak matrix elements first term in (17) gives zero for the point-like nucleus and all value for the matrix elements is given by the second, core polarization term. Even for finite size nucleus, contribution of the first term in (17) is several orders of magnitude smaller than of the second term. This means that \(p – d\) weak matrix elements don’t come from short distances and all arguments based on that assumption are not valid for them.

The \(E_{1PNC}\) amplitude can be presented as a sum of three terms (see eq. (16)). Corresponding numbers for the \(s – d\) PNC amplitudes in Cs, Ba\(^+\), Fr and Ra\(^+\) as well as for the \(6p_{1/2} – 6p_{3/2}\) PNC amplitude in Tl are presented in Table II. The numbers in table are organized in such a way that the term which is proportional to the \(s – p\) weak matrix element goes first, second term is proportional to the \(p – d\) matrix element and the last term has the mix of both. Note that this last term is not included to the sum over single-electron states expression (16). It is small for alkali atoms. However, it is not negligible and we present it here to demonstrate that its inclusion is important for accurate calculations.

The numbers in the table indicate that, as one would expect, term proportional to the \(s – p\) matrix element strongly dominates in the \(E_{1PNC}\) amplitude. However, the term proportional to the \(p – d\) weak matrix element is not small at all and brings significant complications to the behavior of the \(E_{1PNC}\) amplitudes. The case of particular interest is comparison of the \(s – d\) PNC amplitudes of Cs and Ba\(^+\). As one can see from Table II the role of correlations in the Breit correction to these \(E_{1PNC}\) amplitudes is very much different in cases of Cs and Ba\(^+\). Correlations almost do not change Breit correction to the \(s – d\) PNC amplitude in Cs, while they are rather significant in Ba\(^+\).
TABLE III: Effect of Breit interaction on different contributions to the $s - d$ and $p_{1/2} - p_{3/2}$ $E1_{PNC}$ amplitudes in Brueckner approximation ($10^{-11}a_0 e^2 Q_W / N$).

| Atom or ion | Transition | Breit | $\langle \psi_a | H_{E1} + \delta V_{E1} | \delta \psi_b \rangle \sim s - p$ weak m.e. | $\langle \psi_a | H_W + \delta V_W | X_b \rangle \sim p - d$ weak m.e. | $\langle \psi_a | \delta V_{E1W} | \psi_b \rangle$. | Sum |
|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| Cs $5d_{3/2} - 6s_{1/2}$ | no | 3.0045 | 0.8314 | -0.1081 | 3.7277 |
| yes | 2.9846 | 0.8400 | -0.1081 | 3.7165 |
| $\Delta$ | -0.0199 | 0.0086 | 0.0000 | -0.0112 |
| $\Delta$ (%) | -0.66 | 1.0 | 0.0 | -0.30 |
| Ba$^+$ $5d_{3/2} - 6s_{1/2}$ | no | 2.5776 | -0.2486 | -0.1465 | 2.1826 |
| yes | 2.5583 | -0.2469 | -0.1462 | 2.1653 |
| $\Delta$ | -0.0193 | 0.0017 | 0.0003 | -0.0173 |
| $\Delta$ (%) | -0.75 | 0.07 | 0.02 | -0.79 |
| Tl $6p_{3/2} - 6p_{1/2}$ | no | 37.454 | -1.195 | -1.1989 | 24.270 |
| yes | 37.106 | -1.191 | -1.1869 | 24.046 |
| $\Delta$ | -0.348 | 0.004 | 0.120 | -0.224 |
| $\Delta$ (%) | -0.93 | 0.03 | 1.0 | -0.92 |
| Fr $6d_{3/2} - 7s_{1/2}$ | no | 51.598 | 6.466 | -1.627 | 56.437 |
| yes | 51.074 | 6.643 | -1.628 | 56.090 |
| $\Delta$ | -0.524 | 0.177 | 0.001 | -0.347 |
| $\Delta$ (%) | -1.00 | 2.74 | 0.0 | -0.61 |
| Ra$^+$ $6d_{3/2} - 7s_{1/2}$ | no | 46.767 | -1.964 | -2.294 | 42.511 |
| yes | 46.230 | -1.973 | -2.287 | 41.971 |
| $\Delta$ | -0.537 | 0.009 | 0.007 | -0.540 |
| $\Delta$ (%) | -1.15 | 0.46 | 0.31 | -1.27 |

For a more detailed analysis of the $s - d$ PNC amplitudes in Cs and Ba$^+$ we present another set of data in Table IV. This data is similar to those in Table III but in TDHF approximation. Data presented in Table III is in Brueckner approximation which means that correlations are included to all orders in $\Sigma$. In contrast, data from Table IV contains no correlations. Comparison of the data in Table III and Table IV shows that correlation correction to terms proportional to the $s - p$ weak matrix elements is small. This is similar to the $s - s$ PNC amplitude and the same arguments are valid to explain this. On the other hand, correlations significantly increase (by an order of magnitude) the contribution of the terms proportional to the $p - d$ weak matrix elements. Correspondingly, Breit correction also increases. This is also well expected fact given that correlations increase density of external electron in the core. In summary, different behavior of the $s - p$ and $p - d$ weak matrix elements with respect to correlations is due to different distances from which these matrix elements get their values. The $s - p$ matrix elements are well localized at atomic nucleus, while $p - d$ matrix elements localized on much larger distances inside atomic core.

Since correlations have different effect on Breit correction to the $6s_{1/2} - 5d_{3/2}$ PNC amplitude in Cs depending on whether they are included in linear in $\Sigma$ approximation (formula (12)) of in all-order Brueckner approximation (formula (15)), it is important to check that all difference is due to higher order in $\Sigma$ terms. To do this we extract linear in $\Sigma$ contribution from Brueckner approximation and compare it with the result obtained using formula (12). This is done with the use of rescaling procedure similar to those discussed in the end of previous section for the Breit operator. However, this time we rescale correlation potential $\Sigma$. Namely, we replace $\Sigma$ in eqs. (13) and (14) by $S \Sigma$, where $S$ is rescaling parameter. Calculating Breit correction with $S << 1$ and extrapolating it to $S = 1$ leaves only linear in $\Sigma$ contributions. The results are presented in Table V. Extrapolation to $S = 1$ is done using the formula

$$\Delta(S = 1) = \Delta(0) + \frac{\Delta(S) - \Delta(0)}{S}.$$ 

Corresponding numbers are presented in the last column.
TABLE IV: Effect of Breit interaction on different contributions to the $5d_{3/2} - 6s$ PNC amplitude in Cs and Ba$^+$ in TDHF approximation ($10^{-11}ie\alpha BQ_W/N$).

| Atom or ion | Breit (yes/no) | $\langle \psi_{5d_{3/2}} | H_{E1} + \delta \hat{V}_{E1} | \delta \psi_{6s} \rangle_{\sim s - p \text{ weak m.e.}}$ | $\langle \psi_{5d_{3/2}} | H_W + \delta \hat{V}_W | X_{6s} \rangle_{\sim p - d \text{ weak m.e.}}$ | $\langle \psi_{5d_{3/2}} | \delta \hat{V}_{E1W} | \psi_{6s} \rangle$ | Sum |
|-------------|----------------|-------------------------------------------------|-------------------------------------------------|--------------------------------------|-------|
| Cs          | no             | 2.9009                                          | 0.2806                                           | -0.0637                             | 3.1177 |
|             | yes            | 2.8836                                          | 0.2814                                           | -0.0638                             | 3.1012 |
|             | $\Delta$       | -0.0173                                         | 0.0008                                           | 0.0001                              | -0.0165 |
|             | $\Delta$ (%)   | -0.60                                           | 0.29                                             | 0.0                                  | -0.53  |
| Ba$^+$      | no             | 2.6079                                          | -0.3155                                          | -0.1245                             | 2.1678 |
|             | yes            | 2.5886                                          | -0.3131                                          | -0.1242                             | 2.1513 |
|             | $\Delta$       | -0.0193                                         | 0.0024                                           | 0.003                               | -0.0165 |
|             | $\Delta$ (%)   | -0.74                                           | 0.76                                             | 0.2                                 | -0.76  |

TABLE V: Breit correction to the $6s - 5d_{3/2}$ PNC amplitude in Cs in Brueckner approximation as a function of rescaling parameter $S$ ($\hat{\Sigma} \rightarrow S\hat{\Sigma}$ in (13) and (14)) ($10^{-11}ie\alpha BQ_W/N$).

| S           | No Breit with Breit | $\Delta$ | $\Delta(S) - \Delta(0)$ | $\Delta(S = 1)$ |
|-------------|---------------------|----------|--------------------------|-----------------|
| 0.0         | 3.117696            | 3.10125  | -0.016481                | 0               |
| 0.1         | 3.160052            | 3.143462 | -0.016590                | -0.000109       | -0.017571 |
| 0.2         | 3.203363            | 3.186710 | -0.016653                | -0.000172       | -0.017341 |
| 0.4         | 3.295216            | 3.278633 | -0.016583                | -0.000102       | -0.016736 |
| 0.6         | 3.400763            | 3.384702 | -0.016061                | 0.000420        | 0.015781  |
| 0.8         | 3.534769            | 3.520128 | -0.014641                | 0.001840        | 0.014181  |
| 1.0         | 3.727607            | 3.716356 | -0.011251                | 0.005230        | 0.011251  |

of Table IV One can see that the value of Breit correction calculated at $S = 0.1$ and extrapolated to $S = 1$ (-0.017571) practically coincide with the value -0.0176 obtained using formula (12) (see Table I). For larger values of $S$ non-linear in $\hat{\Sigma}$ terms become important and rapidly change the value of Breit correction.

There are few more important conclusions which can be drawn from the fact that Breit correction to a PNC amplitude is only sensitive to change of the electron density. This change of density is proportional to the value of the correlation potential $\hat{\Sigma}$. Therefore, it is important to check how inclusion of some extra terms into $\hat{\Sigma}$ affect the value of the Breit correction to the PNC amplitudes. For example, inclusion of the Breit interaction itself into calculation of $\hat{\Sigma}$ does not change its value very much. Corresponding change of removal energies of Cs is less than 0.02%, while change of the $6s - 6p_{1/2}$ energy interval is 0.04% only. Test calculations show that corresponding change to the PNC amplitude is also small, it is 0.04% for the $6s - 5d3/2$ PNC amplitude and even smaller for the $6s - 7s$ PNC amplitude. On the other hand, it is well known from a number of calculations (see, e.g. 13) that inclusion into $\hat{\Sigma}$ of certain higher-order Coulomb terms leads to significant change in the value of $\hat{\Sigma}$ and electron density on short distances, bring theoretical values for energies, hyperfine structure, transition amplitudes, etc. to much better agreement with the experiment. Therefore, it would be inappropriate to assume a priori that higher-order Coulomb terms do not affect Breit correction. This is to be checked numerically. We have performed such calculations and the results show that the effect of the higher-order Coulomb terms in $\hat{\Sigma}$ is indeed small. Its value is close to the effect of inclusion of Breit interaction into $\hat{\Sigma}$. Moreover, the two effects tend to cancel each other. One can say therefore that inclusion of Breit and higher-order Coulomb terms into $\hat{\Sigma}$ are equally important or unimportant depending of the needed accuracy.

Let us now come back to comparison of the $s - d$ PNC amplitude for Cs and Ba$^+$ for few more important observations. If terms proportional to $s - p$ and $p - d$ weak matrix elements are compared separately, their behavior is very similar for both atoms. This is a natural consequence of the similar electron structure. However, the total $s - d$ PNC amplitude is more sensitive to small difference in the electron structure. In Ba$^+$ ion $5d$ states are lower than the $6p$ states while in Cs $5d$ states are higher than the $6p$ states. This leads to larger correlation correction to the $p - d$ part of the PNC amplitude in Ba$^+$ compared to those of Cs. This also leads to the opposite sign of these terms in Ba$^+$ and Cs. As a result, the effect of correlations on final PNC amplitude is very different. In general, the effect of correlations on $s - d$ and $p_{1/2} - p_{3/2}$ amplitudes is very hard to predict due to different behavior of terms proportional to $s - p$ and $p - d$ weak matrix elements.

Having accurate results for Breit correction to the PNC amplitudes for many atoms we can now check how they rescale with the nuclear charge $Z$. This would allow us to obtain Breit correction for other atoms without doing...
TABLE VI: Breit corrections to the PNC amplitudes in Cs, Ba⁺, Tl, Fr and Ra⁺ (10⁻¹¹ iεaB QW/N), comparison with other calculations.

| Atom | Transition | ΔBreit | Source |
|------|------------|--------|--------|
| Cs 6s - 7s | -0.0056 | this work |
| Cs 6s - 5d₃/₂ | -0.0054 | Derevianko [14] |
| Cs 6s - 5d₃/₂ | -0.0055 | Dzuba et al [17] |
| Cs 6s - 5d₃/₂ | -0.004 | Kozlov et al [8] |
| Cs 6s - 5d₃/₂ | -0.0045 | Shabaev et al [21] |
| Ba⁺ 6s - 5d₃/₂ | -0.0112 | this work |
| Tl 6p₁/₂ - 6p₃/₂ | -0.224 | this work |
| Fr 7s - 8s | -0.15 | this work |
| Fr 7s - 6d₃/₂ | -0.18 | Derevianko [19] |
| Fr 7s - 6d₃/₂ | -0.15 | Safonova and Johnson [20] |
| Ra⁺ 7s - 6d₃/₂ | -0.541 | Shabaev et al [11] |

It is easy to see that Breit correction to similar amplitudes in atoms with similar electron structure is just proportional to \( Z \). For example, \( \Delta E_{PNC}(Fr) = (87/55)\Delta E_{PNC}(Cs) \). It is interesting to note that rescaling from the 6s – 7s amplitude in Cs to the 6p₁/₂ – 6p₃/₂ amplitude in Tl gives result which is very close to the correct answer: \( \Delta E_{PNC}(Tl) = (81/55)\Delta E_{PNC}(Cs) = -0.91\% \) while accurate calculations give \(-0.92\%\). However, this is just fortunate coincidence. Separate analysis of terms proportional to the \( s – p \) and \( p – d \) weak matrix elements show that no reliable rescaling between Cs and Tl is possible. The same is true for any other pair of the PNC amplitudes which correspond to different electron structures.

We present our final results in Table VI together with the results of other authors. The results for the 6s – 7s amplitude in Cs and 7s – 8s amplitude in Fr are in good agreement with other calculations. However, we believe that our results are the most accurate due to non-perturbative treatment of the Breit interaction which is complete up to second order of the MBPT. The results for other atoms as well as for the \( s – d \) PNC amplitudes for Cs and Fr are presented for the first time.

We now can use the result of this work for the Breit interaction contribution and our previous calculations of other contributions to find the PNC amplitude in ¹³³Cs, extract value of the weak charge and compare it with the standard model. Our many-body calculations of the PNC amplitude produced by the electron-nucleus weak interaction gave the following result [17] (without the Breit contribution and QED radiative corrections)

\[
E_{PNC} = -0.9060(1 ± 0.5\%) × 10^{-11} iεa_B(-Q_W/N).
\]

We take the Breit contribution -0.0056 from this work and the QED radiative corrections -0.0029 (-0.32 % of the PNC amplitude) from Ref. [12]. This gives

\[
E_{PNC} = -0.8975(1 ± 0.5\%) × 10^{-11} iεa_B(-Q_W/N).
\]

In the experiment [2] the ratio \( E_{PNC}/\beta \), where \( \beta \) is the vector transition polarizability, actually has been measured. To extract \( Q_W \) we used \( \beta = 26.99(5) a_B^2 \) obtained in [17] as the statistical average of the two most accurate values of \( \beta \). From the measurements of the PNC amplitude [2] we obtain

\[
Q_W = -72.69(29)_{\text{exp}}(36)_{\text{theor}}.
\]

The difference with the standard model value \( Q_W^{SM} = -73.19(3) \) is

\[
Q_W - Q_W^{SM} = 0.50(46),
\]

adding the errors in quadrature. Thus, the difference between the central points is one standard deviation.

For ²⁰⁵Tl we use PNC amplitude from Ref. [16],

\[
E_{PNC} = -(27.0 ± 0.8) × 10^{-11} iεa_B(-Q_W/N),
\]

the QED radiative correction -0.57 % (see details in [1]), the neutron skin correction -0.3 % [22] and the Breit correction -0.92 % from this work. The result is

\[
E_{PNC} = -(26.5 ± 0.8) × 10^{-11} iεa_B(-Q_W/N).
\]

Using M₁ amplitude 1.693 a.u. from [22] and measurement [24] \( \text{Im}(E_{PNC}/M₁) = -(14.68 ± 0.17) \times 10^{-8} \) a.u. we obtain for ²⁰⁵Tl

\[
Q_W = -116.2(1.3)_{\text{exp}}(3.5)_{\text{theor}}.
\]

The standard model value is -116.81(4) [22]. The difference with the standard model for Tl is

\[
Q_W - Q_W^{SM} = 0.6(3.7),
\]

IV. CONCLUSION

We have developed a method of non-perturbative treatment of the Breit interaction in accurate calculations for many-electron atoms. The method has been applied to calculation of the Breit correction to the PNC amplitudes of Cs, Ba⁺, Tl, Fr and Ra⁺. The results for the 6s – 7s amplitude in Cs and 7s – 8s amplitude in Fr are in good agreement with other calculations. The results for other atoms and for the \( s – d \) PNC amplitudes for Cs and Fr are presented for the first time. The following features of the Breit correction to the PNC amplitudes have been revealed:

- The effect of correlations on the \( s – s \) PNC amplitudes is small.
- In contrast, correlations are important for those PNC amplitudes which depend on the \( p – d \) weak matrix elements between valence states.
- For accurate treatment of correlations inclusion of linear in the correlation potential \( \Sigma \) terms is not enough. The main effect is due to the change in density of external electron inside the core which is magnified in higher orders in \( \Sigma \). It can be included by the use of Brueckner orbitals.
• Inclusion of the Breit interaction as well as higher-orders Coulomb terms into correlation potential $\hat{\Sigma}$ have only small effect on PNC amplitudes and can be neglected in most cases.

• Numerical cancellation of the effects of Breit interaction on E1 transition amplitudes and energy denominators in the $s-s$ PNC amplitudes for Cs and Fr is rather fortunate. No such cancellation takes place for other atoms and for the $s-d$ amplitudes of Cs and Fr. The same is probably true for the radiative corrections to the PNC amplitudes.

Rescaling of the Breit correction to the PNC amplitudes using ratio of the nuclear charges $Z$ can only be done to similar amplitudes in atoms with similar electron structure.

Combining Breit corrections to PNC amplitudes in cesium and thallium with previous accurate calculations and measurements confirms good agreement of the weak nuclear charges of these atoms with the prediction of the standard model.

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