Quantum electrodynamics corrections to energies, transition amplitudes and parity nonconservation in Rb, Cs, Ba\(^+\), Tl, Fr and Ra\(^+\).

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(Dated: February 5, 2013)

We use previously developed radiative potential method to calculate quantum electrodynamics (QED) corrections to energy levels and electric dipole transition amplitudes for atoms which are used for the study of the parity non-conservation (PNC) in atoms. The QED shift in energies and dipole amplitudes leads to noticeable change in the PNC amplitudes. This study compliments the previous considered QED corrections to the weak matrix elements. We demonstrate that the QED corrections due to the change in energies and dipole matrix elements are comparable in value to those due to change in weak matrix elements.

PACS numbers: 11.30.Er, 31.30.jg

I. INTRODUCTION

The study of parity nonconservation (PNC) in atoms provides a low-energy search for new physics beyond the standard model (see, e.g. \(^1\)\(^2\)), which is a relatively inexpensive alternative to the high-energy searches performed in colliders. In fact, PNC in cesium is currently the most precise low-energy test of the electroweak theory due to the high accuracy of the measurements \(^3\)\(^4\)\(^5\) and the calculations needed for their interpretation \(^6\) (see also \(^6\)\(^7\)).

The level of precision that has been obtained in atomic physics calculations and measurements has meant that strong-field QED corrections are observable and must be taken into account. It was shown in fact, that the inclusion of self-energy-type QED corrections to PNC calculations in cesium restored the agreement with the standard model \(^10\)\(^12\) (see also \(^13\)\(^15\)). Just as these calculations have proven to be important in the case of cesium, they will be necessary for the calculations of other atoms as the accuracy increases and as new experiments become available. For this reason, using the “radiative potential” method developed in Ref. \(^14\), we present calculations of the QED corrections to the PNC amplitudes of several transitions in Rb, Cs, Ba\(^+\), Tl, Fr and Ra\(^+\).

The case of rubidium is interesting because of its simple electron structure and small value of different corrections to the PNC amplitude \(^8\). The interpretation of the PNC measurements for Rb can be more reliable than for other atoms. We have shown in our previous work \(^8\) that the accuracy of the calculations for rubidium can surpass those for cesium, while the PNC amplitude is only several times smaller \(^8\) (see also \(^10\)\(^16\)).

Francium is a particularly important application. The FrPNC collaboration has begun the construction of a laser cooling and trapping apparatus at the TRIUMF laboratories in Canada with the purpose of measuring atomic parity nonconservation in artificially produced francium \(^17\). With a PNC amplitude expected to be around 15 times larger than that of cesium, and its relatively simple electronic configuration which leads to accurate calculations, francium is an ideal atom for precision measurements of PNC \(^18\)\(^19\)\(^20\). When these measurements become available it will be very important to have accurate atomic calculations for analysis, and these calculations will require contributions from quantum electrodynamics effects.

There are accurate calculations and measurements available for thallium \(^16\)\(^21\)\(^22\), and measurements have also been considered for the Ba\(^+\) ion \(^19\)\(^23\) and are in progress for the Ra\(^+\) ion \(^24\).

II. QED CORRECTIONS

The quantum electrodynamics corrections considered in this work arise from vacuum polarization and electron self-energy. The inclusion of vacuum polarization is numerically relatively simple, achieved via inclusion of the Uehling potential. The self-energy contribution is included via the radiative potential method developed in Ref. \(^14\). Note that the radiative correction to the electric dipole transition operator \(d_{E1}\) (vertex correction) is very small and may be neglected. The change of the electric dipole matrix elements come from the QED corrections to the electron wave functions.

The parity nonconservation amplitude of a transition \((a \rightarrow b)\) between states of the same parity can be expressed via the sum over all possible intermediate opposite parity states \(n\),

\[
E_{PNC} = \sum_n \left[ \frac{\langle b|d_{E1}|n\rangle\langle n|\hat{h}_W|a\rangle}{E_a - E_n} + \frac{\langle b|\hat{h}_W|n\rangle\langle n|d_{E1}|a\rangle}{E_b - E_n} \right],
\]

(1)

where \(d_{E1}\) is the electric dipole transition operator and \(\hat{h}_W\) is the nuclear-spin-independent weak interaction.
TABLE I: Values (from Ref’s [10–12]) for the percentage contributions of vacuum polarization including the Uehling and smaller Wichmann-Kroll (W-K) potentials, and self-energy-vertex (SE-V) to weak s-p matrix elements for various atoms. Uncertainty is estimated from the spread of values of different sources.

|        | Uehling | SE-V | W-K | Total |
|--------|---------|------|-----|-------|
| Rb     | 0.20    | -0.51| 0.001 | -0.31(2) |
| Cs     | 0.40    | -0.84| 0.003 | -0.43(3) |
| Ba⁺    | 0.41    | -0.86| 0.003 | -0.45(3) |
| Tl     | 0.93    | -1.44| 0.015 | -0.50(5) |
| Fr     | 1.13    | -1.75| 0.02  | -0.60(7) |
| Ra⁺    | 1.17    | -1.80| 0.02  | -0.61(7) |

We consider QED corrections from the three sources separately – corrections to the weak amplitudes, the dipole amplitudes and the energy denominators.

In the original works, QED corrections were only calculated for the weak matrix elements (see e.g. [10–13]). This was a reasonable approximation numerically for cesium due to a chance cancellation between QED contributions coming from corrections to the energy levels and dipole matrix elements, which were calculated by Flambaum and Ginges [14]. This cancellation is not guaranteed and it was demonstrated in Ref. [14] that corrections from all three sources are equally important and must be included. Full determinations of QED corrections to the entire PNC amplitude have only been considered for cesium [8, 14, 15].

The radiative potential method, developed by Flambaum and Ginges [14], defines an approximate potential \( \delta \hat{L} \) such that the radiative correction to the energies coincides with its average value,

\[
\delta E_n = \langle n | \delta \hat{L} | n \rangle.
\]

This potential takes into account the local vacuum polarization operator (including the lowest-order in \( Z \alpha \) Uehling potential as well as the higher order Wichmann-Kroll potential) and the non-local strong Coulomb field electron self-energy operator.

In this work, we use the existing calculations of QED corrections to the weak matrix elements, which are presented in Table I. These values have been taken from the works Ref’s [10–12] (see also [13]). Midpoints and uncertainties have been chosen to agree with different previous determinations. Note also that these calculations are valid only for s-p \( 1/2 \) weak transitions.

We then use the radiative potential method outlined above, with the exception of the small Wichmann-Kroll term, to calculate the QED corrections to the energy levels and electric dipole matrix elements. We then calculate the dominating terms in equation (1) with and without the radiative corrections to determine the total percentage correction to the PNC amplitudes for several transitions in Rb, Cs, Ba⁺, Tl, Fr and Ra⁺.

III. CALCULATIONS

We use the sum-over-states approach to calculate the PNC amplitudes. Relativistic Hartree-Fock (RHF) method is used to construct single-electron orbitals and random phase approximation (RPA) is used to include the effect of core polarization by external fields.

Core-valence correlations are included by means of the correlation potential method (CPM) [25]. The second-order correlation potential \( \hat{\Sigma}^{(2)} \) is calculated using many-body perturbation theory and then used to construct the so-called Brueckner orbitals (BO) for the external electron. BO are found by solving the Hartree-Fock-like equations with an extra operator \( \hat{\Sigma} \):

\[
(\hat{H}_0 + \hat{\Sigma}^{(2)} - E_n)\psi_n^{(BO)} = 0,
\]

where \( \hat{H}_0 \) is the relativistic Hartree-Fock Hamiltonian and index \( n \) denotes valence states. The BO \( \psi_n^{(BO)} \) and energy \( E_n \) include correlations.

We then use a simple scaling procedure to estimate the contribution of higher-order correlations by including a factor in front of the correlation potential, \( \lambda \hat{\Sigma}^{(2)} \), which is chosen to reproduce energy levels of the lowest lying valence states. A separate \( \lambda \) is used for each of the initial/final states, and another is used for each set of intermediate states (e.g. \( np_{1/2}, np_{3/2} \)). For the second-order correlation potential, values for the fitting parameter typically take values \( \lambda \sim 0.8 \sim 0.9 \). This fitting generally increases the accuracy of the wave-functions and therefore the matrix elements.

The PNC amplitude is given by the expression similar to (1), in which states \( a, b, n \) are single-electron RHF states, and operators \( \hat{d}_{E1} \) and \( \hat{h}_W \) are modified to include the effect of core polarization: \( \hat{d}_{E1} \rightarrow \hat{d}_{E1} + \delta \hat{V}_{E1} \), \( \hat{h}_W \rightarrow \hat{h}_W + \delta \hat{V}_W \). Here \( \delta \hat{V}_f \) is the correction to the self-consistent core potential due to the effect of external field \( f \) (\( f \) is either electric field of laser light \( \hat{d}_{E1} \) or weak electron-nucleus interaction \( \hat{h}_W \)). The corrections to the core potential are found by solving self-consistently the RPA equations for the core states

\[
(\hat{H}_0 - \varepsilon_c)\delta \psi_c = -(\hat{f} + \delta \hat{V}_f)\psi_c.
\]

Here \( \hat{H}_0 \) is the RHF Hamiltonian, index \( c \) numerates core states, \( \hat{f} \) is the operator of external field (weak or electric dipole).

QED corrections are included by adding the radiative potential to the RHF Hamiltonian \( \hat{H}_0 \). This is done on the stages of calculating single-electron RHF and Brueckner orbitals and solving the RPA equations for the electric dipole field. We remind the reader that we don’t include QED corrections for the weak interaction. The more reliable results for weak matrix elements are found in different approaches considered before in Refs. [10–13].

B-spline technique [26] is used to construct sets of single-electron orbitals used in the calculate \( \hat{\Sigma}^{(2)} \) and for summation in (1). The basis states used to calculate
\[ \sum^{(2)} \] are the linear combinations of B-splines which are the eigenstates of the RHF Hamiltonian \( \hat{H}_0 \) (RHF orbitals). The basis states used in the summation \( \{ \) are the eigenstates of the \( \hat{H}_0 + \sum^{(2)} \) Hamiltonian (Brueckner orbitals).

The approach described above does not take into account the effect of core polarization due to simultaneous action of the weak and electromagnetic interactions. An example of the contribution of this type is presented on Fig. 1 for the case of thallium. The contribution of the double core polarization to all PNC amplitudes considered in present paper except thallium does not exceed one per cent. Therefore, it can be neglected in calculating the effect of core polarization due to simultaneous action of the weak and electromagnetic interactions. An example of the contribution of this type is presented on Fig. 1 for the case of thallium. The contribution of the double core polarization to all PNC amplitudes considered in present paper except thallium does not exceed one percent. Therefore, it can be neglected in calculating the effect of core polarization due to simultaneous action of the weak and electromagnetic interactions.

The latter are taken from previous works [10–12] (see also Table I). Values given in units of \( \times 10^{-15} \) a.u. are the fine structure constant.

\[ \langle b|\hat{d}_{E1}|a\rangle = \langle b|\hat{d}_{E1}|a\rangle_0 (1 + \frac{\alpha}{\pi} R_{E1}), \]

where the subscript 0 indicates the zeroth order matrix element, without radiative corrections, and \( \alpha \) is the fine structure constant.

\[ E_{1}\text{ transitions in the RPA and fitted second-order Brueckner (BO)} \]

\begin{table}[h]
\centering
\begin{tabular}{|c|c|c|c|}
\hline
Transition & This work & Previous calculations \\
& (RPA + BO) & \text{ Previous calculations} \\
\hline
\( ^{85}\text{Rb} \) & 5s-6s & 0.139 & 0.139 [6] \\
& 5s-4d_{3/2} & 0.449 & — \\
\hline
\( ^{133}\text{Cs} \) & 6s-7s & 0.897 & 0.8977 [5] \\
& 6s-5d_{3/2} & 3.75 & 3.76 [19] \\
\hline
\( ^{138}\text{Ba}^+ \) & 6s-7s & 0.671 & — \\
& 6s-5d_{3/2} & 2.36 & 2.34 [19] \\
\hline
\( ^{223}\text{Fr} \) & 7s-8s & 15.4 & 15.41 [20] \\
& 7s-6d_{3/2} & 59.4 & 59.5 [19] \\
\hline
\( ^{226}\text{Ra}^+ \) & 7s-8s & 10.9 & — \\
& 7s-6d_{3/2} & 46.6 & 45.9 [19] \\
\hline
\end{tabular}
\end{table}

\[ \text{IV. RESULTS AND DISCUSSION} \]

Percentage QED corrections to individual lowest energy levels are presented in Table IV and corrections \( R_{E1} \) to dipole matrix elements are presented in Table IV. The factor \( R_{E1} \) is defined

\[ \langle b|\hat{d}_{E1}|a\rangle = \langle b|\hat{d}_{E1}|a\rangle_0 (1 + \frac{\alpha}{\pi} R_{E1}), \]

where the subscript 0 indicates the zeroth order matrix element, without radiative corrections, and \( \alpha \) is the fine structure constant.

Tables III and IV show QED corrections to the lowest states only. However, we include QED corrections to all states used in the summation \( \{ \). The results are presented in Table IV together with the correction arising from the QED correction to the weak matrix elements. The latter are taken from previous works [10–12] (see also Table I).

While there is typically still some cancellation between the contributions from the energy levels and dipole matrix elements in the transitions studied, it is not always as complete as it is with cesium, making these results significant.

Despite the fact that there are some individual corrections in the atoms that are quite large, there is significant cancellation between contributions from the weak matrix elements and the combined contributions from the energies and dipoles in most of the transitions presented. This
TABLE III: Percentage QED corrections to ionization energies of lowest states for several atoms.

| Atom | 5s | 6s | 6p$_{1/2}$ | 6p$_{3/2}$ | 6d$_{3/2}$ | 6p$_{3/2}$ |
|------|----|----|----------|----------|----------|----------|
| Rb   | -0.40 | 0.023 | 0.003   | 0.002     | 0.003     | 0.001    |
| Cs   | 0.069 | -0.040 | 0.006   | 0.004     | 0.003     | 0.031    |
| Ba$^+$ | 0.055 | -0.035 | 0.005   | 0.004     | 0.003     | 0.028    |
| Tl$^a$ | 0.01 | -0.02 | -0.14   | -0.07     |           |          |
| Fr   | -0.142 | -0.076 | 0.002   | 0.001     | 0.067     | -0.003   |
| Ra$^+$ | -0.109 | -0.066 | 0.001   | 0.000     | 0.059     | -0.005   |

$^a$V$^N=3$ approximation

TABLE IV: QED corrections $R_{E1}$ to the dipole matrix elements of several atoms. $R_{E1}$ is defined in equation (4).

| Atom | Transition | $R_{E1}$ |
|------|------------|----------|
| Rb   | 5s-5p$_{1/2}$ | 0.193 |
| Cs   | 6s-6p$_{1/2}$ | 0.328 |
| Ba$^+$ | 6s-6p$_{1/2}$ | 0.257 |
| Tl$^a$ | 6p$_{1/2}-6p$_{3/2}$ | 0.619 |
| Fr   | 7s-7p$_{1/2}$ | 0.047 |
| Ra$^+$ | 7s-7p$_{3/2}$ | 0.483 |

$^a$V$^N=3$ approximation

causes the total QED corrections in most atoms to be highly suppressed.

The uncertainty of the total QED corrections to the PNC amplitudes comes from uncertainties of all three sources ($H_W$, $E_n$ and $E1$) added in quadrature. The uncertainty of the first term ($H_W$) has been estimated in [10-12]. The estimation of uncertainties for two other terms ($E_n$ and $E1$) comes from the spread of values of the QED correction found in different approximations (RPA, Brueckner, etc.).

TABLE V: QED corrections (as percentages) to PNC amplitudes for several atoms. Corrections due to weak matrix elements ($H_W$) are taken from Table IV. Corrections due to change of energy denominators ($E_n$) and electric dipole transition amplitudes ($E1$) are the result of present work.

| Transition | $H_W$ | $E_n$ | $E1$ | Total |
|------------|-------|-------|------|-------|
| Rb 5s-6s  | -0.31 | -0.25 | 0.31 | -0.25(4) |
| 5s-4d$_{3/2}$ | -0.31 | 0.12  | 0.001 | -0.19(5) |
| Cs 6s-7s  | -0.43 | 0.04  | 0.52 | -0.33(4) |
| 6s-5d$_{3/2}$ | -0.43 | 0.20  | 0.003 | -0.23(7) |
| Ba$^+$ 6s-7s | -0.45 | -0.54 | 0.68 | -0.31(4) |
| 6s-5d$_{3/2}$ | -0.45 | 0.29  | 0.05  | -0.22(8) |
| Tl 6p$_{1/2}-6p$_{3/2}$ | -0.50 | 0.07  | 0.06  | -0.37(8) |
| Fr 7s-8s  | -0.60 | -0.83 | 1.02 | -0.41(8) |
| 7s-6d$_{3/2}$ | -0.60 | 0.42  | -0.02 | -0.2(1) |
| Ra$^+$ 7s-8s | -0.61 | -0.97 | 1.20 | -0.38(9) |
| 7s-6d$_{3/2}$ | -0.61 | 0.47  | -0.09 | -0.2(1) |

a. Acknowledgments — This work was supported in part by the Australian Research Council.

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