High-Accuracy Calculation of $6s \rightarrow 7s$ Parity-Nonconserving Amplitude in Cs

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We calculated the parity-nonconserving (PNC) $6s \rightarrow 7s$ amplitude in Cs. In the Dirac-Coulomb approximation our result is in good agreement with other calculations. Breit corrections to the PNC amplitude and to the Stark-induced amplitude β are found to be -0.4% and -1%, respectively. The weak charge of ^{133}Cs is $Q_W = -72.5 \pm 0.7$ in agreement with the standard model.

Introduction.—The last and most accurate measurement of the ratio of the parity-nonconserving (PNC) amplitude in Cs to the Stark-induced amplitude β was done in Boulder [1]. Later the amplitude β was measured with a very high accuracy [2]. These measurements together with atomic calculations of the PNC amplitude [3,4] gave the most accurate atomic test of the standard model. The authors of the calculations [3,4] estimated their accuracy to be 1%. After that Bennett and Wieman [2] compared theoretical and experimental results for a number of observables including hyperfine constants, $E1$ amplitudes, and the Stark-induced amplitude β and suggested that the actual accuracy of atomic calculations of the PNC amplitude was 0.4%. Their analysis gave the following value of the weak charge of ^{133}Cs: $Q_W = -72.06(44)$, where experimental and theoretical errors are added in quadrature. That differs by 2.3σ from the standard model prediction [5]:

$$Q_W^{\text{SM}} = -73.09(3).$$

This result caused an intensive discussion (see [6], and references therein). It also stimulated a new wave of atomic calculations [7–9]. First Derevianko [7] suggested that previous calculations underestimated the Breit correction. He calculated the latter and added it to the PNC amplitude from [3,4]. That reduced the discrepancy to 1.0σ. Somewhat smaller Breit corrections were obtained in [8,9].

Here we reanalyze the role of Breit interaction (we consider only the dominant magnetic part of the Breit operator) in calculation of the PNC amplitude in Cs. In contrast to the paper [7] we made a full scale calculation which partly accounts for the higher order corrections of the many-body perturbation theory (MBPT). The Breit interaction was included on all stages of the calculation, i.e., on the stage of the solution of the Dirac-Fock equations, then on the stage of the solution of the random phase approximation (RPA) equations, and, finally, on the stage of the evaluation of the self-energy operator. All these corrections are of the same order of magnitude, which is not surprising taking into account that both RPA and MBPT

contributions to the answer are quite significant. Our final value of Breit correction to the PNC amplitude is -0.4% in agreement with our preliminary result [8].

We also calculated the Breit correction to the Stark-induced amplitude $\beta_{6s,7s}$ and found it to be about 1%. That suggests that an excellent agreement between the theory [4] and the experiment [2] for this constant may be partly accidental. At the end of this paper we discuss corrections, which are not included in PNC calculations and conclude that the accuracy of the atomic theory is close to 1%. Within this accuracy there is no contradiction with the standard model.

Details of the calculation.—The Dirac-Fock equations were solved on a radial grid with the help of the code [10] and all MBPT calculations were done using summations over the basis set. We formed the Dirac-Fock-Coulomb (DFC) and the Dirac-Fock-Coulomb-Breit (DFCB) variants of the basis set and repeated all calculations in exactly the same way for both of them.

It is known from previous calculations of PNC effects in Cs that high orders in the residual Coulomb interaction are very important. Indeed, the MBPT effects account for 13% of the ionization potential, for more than 60% of the hyperfine constants, and for 22% of the PNC amplitude. Here we calculated explicitly only the second order diagrams but introduced screening coefficients C_k for the Coulomb lines in these diagrams [11]. The latter can be calculated as an average screening of the two electron Coulomb radial integrals of a given multipolarity k. These coefficients served as an approximation to the insertion of the polarization operator in Coulomb lines. The coefficients C_k were chosen as follows: $C_0 = C_1 = 0.85$, and $C_k = 1$ for $k \geq 2$. With these screening coefficients the Brueckner energies of the orbitals appeared to be within 1% from the experimental values. Still the additional corrections were necessary in order to reach the accuracy better than 1%. Thus, we used the energy dependence of the self-energy operator $\sigma(\varepsilon)$ to improve the agreement between calculated energy and the experiment. The optimal one-electron energies ε appeared to be close to the Brueckner energies of

corresponding orbitals. In a similar way we chose the energies in the RPA equations for hyperfine and PNC interactions.

The optimal choice of the one-electron energies for $\sigma(\varepsilon)$ and for RPA matrix elements allowed us to improve the accuracy for the lower part of the spectrum and for the hyperfine constants. Corresponding corrections were smaller than 1% for the energies and 1%–2% for the hyperfine constants. RPA corrections to the $E1$ amplitudes were much smaller and we did not do any fitting for them. The RPA equations for weak interaction H_P were solved for the same energies as were used for hyperfine constants. That increased PNC amplitude by 1%.

All observables were calculated using Brueckner orbitals and RPA amplitudes. We also calculated two smaller MBPT corrections to the amplitudes. One of them is the so-called structural radiation and the other is the normalization correction [3,4]. The former is typically of the order of a few percent and the latter reduces the final answer by approximately 1%. There are several corrections to the PNC amplitude of the same order of MBPT as these ones. They correspond to the RPA-type diagrams and to the structural radiation-type diagrams with both $E1$ and PNC vertexes on the inner lines. These corrections were shown to be negligible [3,4] and we omitted them here.

Breit interaction for valence electrons.—The frequency independent Breit interaction between electrons 1 and 2 has the form

$$V_B \equiv V_B^1 + V_B^2$$
$$= -\frac{\boldsymbol{\alpha}_1 \cdot \boldsymbol{\alpha}_2}{r_{12}}$$
$$+ \frac{1}{2}\left\{\frac{\boldsymbol{\alpha}_1 \cdot \boldsymbol{\alpha}_2}{r_{12}} - \frac{(\boldsymbol{r}_{12} \cdot \boldsymbol{\alpha}_1)(\boldsymbol{r}_{12} \cdot \boldsymbol{\alpha}_2)}{r_{12}^3}\right\}, \quad (1)$$

where $\boldsymbol{\alpha}_i$ are Dirac matrices and $\boldsymbol{r}_{12}$ is the distance between the electrons. The operator V_B^1 is called the magnetic or Gaunt term, and the operator V_B^2 is called the retardation term. For valence electrons the Gaunt term is known to be about an order of magnitude larger than the second one [12]. The latter is of the same order as the frequency dependent corrections to the operator (1) and as other QED corrections [13]. Therefore, below we neglect the retardation term in Eq. (1).

Calculations of Cs are done in the V^{N-1} approximation and one needs to calculate Breit interaction between the electron and the closed shells only. It is easy to show that in this case only the exchange term of the Breit interaction does not turn to zero. This is almost obvious because for a closed shell $\langle\boldsymbol{\alpha}\rangle = 0$. The exchange Breit interaction can be included in calculation either perturbatively or self-consistently. The core relaxation results in a screening of Breit interaction between the innermost core shells and the valence electron, significantly reducing the final Breit corrections [12,14]. Account for that effect is vital, for example, in the calculations of the multiply charged ions, where Breit corrections are large [15].

In the self-consistent approach, the potential V_B^{core} should be included in the Dirac-Fock equations. For this purpose we modified the Dirac-Fock code [10] to allow for the Coulomb-Breit potential. The self-consistent approach for such observables as hyperfine constants or PNC amplitudes requires the solution of the RPA equations. There are two types of Breit corrections to these equations. First, one has to use DFCB orbitals and DFCB orbital energies in RPA equations. Second, it is necessary to include Breit interaction explicitly in two-electron matrix elements. These types of corrections are of the same order of magnitude and should be included on equal footing.

Finally, we calculated the self-energy operator also using DFCB orbitals and orbital energies. Here we did not include Breit correction to two-electron matrix elements in diagrams for the self-energy. These diagrams arise in the second order in residual Coulomb interaction and always include two Coulomb lines. If in one of these lines the Coulomb interaction is changed to the Breit one, the resultant correction appears to be very small. The reason is that main Coulomb corrections are associated with the interaction of the valence electrons with the upper core shells, while the most important Breit interaction is with the innermost core shells.

All calculations with the exception for structural radiation and normalization corrections were repeated 2 times in exactly the same manner in Dirac-Coulomb and Dirac-Coulomb-Breit approximations. That allowed us to single out Breit corrections even when they were comparable to the errors caused by the incompleteness of the basis set or by the approximations we used to account for higher order terms of MBPT.

Numerical results.—The PNC amplitude of the $6s \rightarrow 7s$ transition can be written as

$$E1_{PNC}(6s, 7s) = \sum_n \left(\frac{\langle 7s_j, m|E1|np_j, m\rangle\langle np_j, m|H_P|6s_j, m\rangle}{\varepsilon_{6s_j} - \varepsilon_{np_j}} + \frac{\langle 7s_j, m|H_P|np_j, m\rangle\langle np_j, m|E1|6s_j, m\rangle}{\varepsilon_{7s_j} - \varepsilon_{np_j}}\right), \quad (2)$$

where $j = 1/2$. This amplitude is sensitive to the energy spectrum and $E1$ amplitudes as well as to the matrix elements of the weak interaction H_P. The latter depends on the wave function in the vicinity of the nucleus and in this respect is similar to the matrix elements of the hyperfine interaction. Thus, in order to estimate the accuracy of the calculation of the PNC amplitude one has to analyze the accuracy for all these observables.

Tables I and II present our results for the energies and hyperfine constants of the lower levels of Cs. These tables

TABLE I. Binding energies for the lower levels of Cs (a.u.). The columns DF and BA correspond to the Dirac-Fock and Brueckner approximations. The column OE corresponds to Brueckner approximation with self-energy calculated at "optimal" energies $\varepsilon(6s) = -0.22$, $\varepsilon(7s) = -0.15$, and $\varepsilon(np) = -0.10$. Finally we give Breit corrections to the energy in Brueckner approximation.

	DF	BA	OE	Breit	Expt.
$6s_{1/2}$	0.127 37	0.144 24	0.143 12	0.000 02	0.143 10
$6p_{1/2}$	0.085 62	0.092 26	0.092 17	−0.000 04	0.092 17
$6p_{3/2}$	0.083 79	0.089 67	0.089 59	−0.000 01	0.089 65
$7s_{1/2}$	0.055 19	0.058 69	0.058 64	0.000 00	0.058 65
$7p_{1/2}$	0.042 02	0.043 89	0.043 86	−0.000 01	0.043 93
$7p_{3/2}$	0.041 37	0.043 05	0.043 03	0.000 00	0.043 10

show results on the different stages of calculation including the initial Dirac-Fock approximation, the MBPT, and the Breit corrections. We also give corrections associated with the optimization of the energies in MBPT and RPA calculations as described above. Calculations were done for the uniformly charged nucleus of the radius 6.20 fm and the uniform magnetic distribution inside the nucleus.

Breit corrections to $E1$ amplitudes appear to be mostly smaller than 0.1%. Similar corrections to scalar polarizabilities of the levels $6s$ and $7s$ are about −0.1%. These polarizabilities can be used to calculate the Stark shift $\delta\nu_{6s,7s}$ for the $6s \rightarrow 7s$ transition [in Hz/(V/cm)^2]:

$$\delta\nu_{6s,7s} = \begin{cases} 0.7268, & \text{without Breit,} \\ 0.7259, & \text{with Breit,} \\ 0.7223, & \text{theory [4],} \\ 0.7262(8), & \text{experiment [16].} \end{cases} \quad (3)$$

Breit correction to the Stark-induced vector amplitude $\beta_{6s,7s}$ is more important because this amplitude turns to zero in the nonrelativistic approximation. Numerical values for this amplitude in a.u. are

$$\beta_{6s,7s} = \begin{cases} 27.17, & \text{without Breit,} \\ 26.89, & \text{with Breit,} \\ 27.0(2), & \text{theory [4],} \\ 27.02(8), & \text{experiment [16].} \end{cases} \quad (4)$$

In the experiment [16] the amplitude β was measured relative to the hyperfine $M1$ amplitude. Dzuba and Flambaum suggested [17] that the latter is slightly smaller than was assumed in [16] and gave the value $\beta = 26.96(5)$.

TABLE II. Hyperfine constants for ^{133}Cs (MHz). Notations are the same as in Table I.

	DF	MBPT	OE	Breit	Theory	Expt.
$6s_{1/2}$	1424	2349	−52	+5.0	2302	2298
$6p_{1/2}$	160.9	298.9	−5.3	−0.2	293.5	292
$6p_{3/2}$	23.9	53.5	−2.3	−0.0	51.2	50.3
$7s_{1/2}$	391.4	546.8	−0.8	+0.8	546.8	546
$7p_{1/2}$	57.6	94.2	−0.2	−0.0	94.0	94.3
$7p_{3/2}$	8.6	17.1	−0.0	−0.0	17.1	· · ·

Our results for the PNC amplitude are presented in Table III. Following [7,18] we introduced −0.1% correction to account for the difference in neutron and charge radii of the nucleus. A somewhat larger correction follows from nuclear calculation [19].

We see that *ab initio* calculation and calculation with "optimal" energies for the self-energy operator and for RPA amplitudes differs by 1%, i.e., PNC amplitude appears to be less sensitive to the variation of the energies used for the self-energy operator $\sigma(\varepsilon)$ and for RPA equations than the hyperfine constants. Thus, we assume that uncertainty for the PNC amplitude associated with the fitting is smaller than for the hyperfine constants.

Discussion.—For the Dirac-Coulomb approximation our value for the PNC amplitude is in good agreement with the results of the calculations [3,4]. Our Breit correction is 2 times smaller than the final result of Derevianko, but we are in good agreement with his result, which includes Breit contribution to the energies of atomic levels and with Dzuba *et al.* (see Table III). Derevianko argues that this correction should not be included if one fits the energies semiempirically.

We first want to note that calculations [3,4] did not use any energy fit. Therefore, Breit correction to these calculations should definitely include this contribution. In our calculation we *did* use the energy fit and thus Derevianko's argument seems to work here. However, we did not insert experimental energies into Eq. (2). Instead, we modified the MBPT by changing the argument of the self-energy operator $\sigma(\varepsilon)$. That changed the energies *and* the Brueckner orbitals thus affecting the numerators as well as the denominators in Eq. (2). We think that this is a more consistent way to account for the high orders of the MBPT. We repeated the energy fit after Breit interaction was included. That changed Breit corrections to different contributions to the PNC amplitude, but the overall correction still remained −0.4%.

The analysis of the numerical data from Tables I and II and Eqs. (3) and (4) shows that the energies, the Stark shift $\delta\nu$, and even the Stark-induced amplitude β are in very good agreement with the experiment. However, the accuracy for the hyperfine constants of the levels $6s$ and $6p_{1/2}$ is significantly lower. In order to improve these constants we had to make the energy fit which changed both constants by approximately 2%. The reason for the low accuracy here is obvious: the MBPT corrections to $A(6s)$ and $A(6p_{1/2})$ are 65% and 81% correspondingly. The MBPT correction to the PNC amplitude is only 22% and the energy fit changes this amplitude only by 1%. Therefore, we estimate our accuracy for the PNC amplitude to be about 0.5%.

This estimate does not include uncertainties associated with the nuclear structure and QED corrections. QED corrections to the hyperfine structure and the uncertainties associated with the nuclear magnetic moment distribution were discussed in [20–22]. The authors conclude that there are several corrections on the scale of 0.1%–0.3%.

TABLE III.   PNC amplitude $E1_{PNC}$ for $6s \rightarrow 7s$ transition in the units $i \times 10^{-11} Q_W/(-N)$ a.u.

	DF	MBPT	OE	Breit	Total
This work	−0.742	−0.896	−0.905	0.004	−0.901
Dzuba *et al.* [3]				⋯	−0.908
Blundell *et al.* [4]			−0.907	0.002	−0.905
Derevianko[a] [7]				0.008	
Derevianko[b] [7]				0.005	
Dzuba *et al.* [9]	−0.739		−0.907	0.005	−0.902

[a]Without Breit corrections to energies.
[b]Including Breit corrections to energies.

For the PNC amplitude the vacuum polarization correction was estimated in [23,24] to be 0.2%–0.4% for $Z = 55$. The core relaxation can screen it significantly, as it does with the Breit correction, so it is rather an order of magnitude estimate of the QED corrections to the PNC amplitude. An uncertainty 0.1%–0.3% is caused by the poor knowledge of the neutron distribution in the nucleus [7,18,19].

In our analysis we use Gaunt approximation to the Breit operator while in the papers [7,9] the retardation term was also included. This may explain the difference between our value 0.004 and the value 0.005 obtained in [9]. The retardation term is of the same order of magnitude as the frequency dependent corrections to the Breit operator and as other QED corrections. Therefore, the difference between our results can serve as an estimate of the accuracy of Breit approximation. Thus, the total uncertainty for the PNC amplitude is about 1% and there is no meaningful difference with the standard model. Our final value for the weak charge is

$$Q_W = -72.5(7).$$

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