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Polarizabilities and parity nonconservation in the Cs atom and limits on the deviation from the standard electroweak model

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A semiempirical calculation of the $6s$-$7s$ Stark amplitude α in Cs has been performed using the most accurate measurements and calculations of the electromagnetic amplitudes available. This is then used to extract the parameters of the electroweak theory from experimental data. The results are $\alpha=269.0(1.3)a_0^3$, weak charge of Cs $Q_W=-72.41(25)_{expt}(80)_{theor}$, deviation from the standard model $S=-1.0(.3)_{expt}(1.0)_{theor}$ and the limit on the mass of the extra Z boson in the SO(10) model $M_{Z_x}>550$ GeV. [S1050-2947(97)50212-5]

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Experiments suggested in [1] for measuring parity nonconservation (PNC) in heavy atoms have provided an important confirmation [2–5] of the standard model of elementary particles. Combining the very accurate recent measurements of parity nonconservation in the Cs atom [5] with theoretical calculations [6,7] gives one a possibility to study new physics beyond the standard model. The measured nuclear spin-independent part of the PNC effect in Cs [5] is of the form (we use the analysis from [8])

$$-\frac{\mathrm{Im}(E_{PNC})}{\beta}=1.5939(56)\frac{\mathrm{mV}}{\mathrm{cm}}, \tag{1}$$

where E_{PNC} is the PNC $E1$ amplitude of the $6s$-$7s$ transition and β is the vector polarizability of the transition. The theoretical values of E_{PNC} are as follows:

$$E_{PNC}=-i|e|a_0 10^{-11}\left(-\frac{Q_W}{N}\right)\times\begin{cases}0.908(10) & \text{(Ref. [6])},\\ 0.905(9) & \text{(Ref. [7])}.\end{cases} \tag{2}$$

Here, Q_W is the weak charge of the cesium nucleus and N is the number of neutrons.

The method for *ab initio* calculations of E_{PNC} that we used in [6] was based on an all-orders summation of the dominating diagrams of the many-body perturbation theory in the residual Coulomb interaction using a relativistic Hartree-Fock basis set and Green's functions. This technique has been described in [6,9].

We took into account direct and exchange polarization of the atomic core by the external electric field and the weak nuclear potential using the time-dependent Hartree-Fock method (summation of the ''RPA with exchange'' chain of diagrams), and calculated second-order correlation corrections and three series of dominating higher-order diagrams:

(i) Screening of the electron-electron interaction. This is a collective phenomenon and so the corresponding chain of diagrams is enhanced by a factor approximately equal to the number of electrons in the external closed subshell (the $5p$ electrons in Cs). We stress that our approach takes into account screening diagrams with double, triple, and higher core electron excitations [10] in contrast to popular pair equations (coupled-cluster) method, where only double excitations are considered.

(ii) Hole-particle interaction. This effect is enhanced by the large zero-multipolarity diagonal matrix elements of the Coulomb interaction.

(iii) Iterations of the self-energy operator (''correlation potential''). This chain of diagrams describes the nonlinear effects of the correlation potential and is enhanced by the small denominator, which is the energy for the excitation of an external electron (in comparison with the excitation energy of a core electron).

The error in the theoretical value was tested in many different ways: by estimating the contribution of the unaccounted higher-order diagrams and by comparing the calculated and measured values of the energy levels, the fine and hyperfine structure intervals, the probabilities of electromagnetic transitions, etc. (see Ref. [6]). The result for the PNC amplitude almost did not change when we introduced factors into the correlation potential to fit the energy levels (in imitation of the unaccounted higher-order diagrams). Important tests of our method included predictions of the spectrum [11] and electromagnetic transition amplitudes for the Fr atom [12], which is an analogue of the Cs atom. Recently, the positions of many energy levels [13] and some transition rates [14] of Fr were measured and found to be in excellent agreement with our predictions.

Our calculations of PNC for atoms with electron structures that are more complex than those of the alkaline atoms were proved to be accurate as well. In a series of works done about ten years ago we claimed an accuracy of 3% for Tl [15], 8% for Pb, and 11% for Bi [16]. All these PNC effects were recently measured to within an accuracy of about 1% [4] and found to be in good agreement with our predictions. This means that our estimates for the theoretical accuracy were correct and probably even too pessimistic. For example, in our first calculation of the Fr energy levels [11] we claimed the accuracy of our predictions to be about 0.5% while the actual agreement with latter measurements was

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found to be 0.1%. The situation was similar for the electromagnetic transitions $6s$-$6p_{1/2}$ and $6s$-$6p_{3/2}$ in Cs (see below). These numerous tests give us firm ground to believe that the theoretical error in E_{PNC} (2) indeed does not exceed 1%.

As can be seen from Eq. (1), an accurate value of the vector transition polarizability β is also required for the interpretation of the PNC measurements. There are no direct experimental measurements of β and so the value $\beta=27.0(2)a_0^3$ calculated in [17] was used for the interpretation of the PNC measurements. The theoretical ratio of the scalar transition polarizability $\alpha=-268(3)a_0^3$ to β $(\alpha/\beta)_{theor}=-9.93(14)$ [17] was in good agreement with the corresponding experimental value $(\alpha/\beta)_{expt}=-9.9(1)$ [18] available at that time. Since then the ratio (α/β) was remeasured with a very high accuracy: $(\alpha/\beta)=-9.905(11)$ [19]. There have also been very precise measurements of the lifetimes of the $6p_{1/2}$ and $6p_{3/2}$ states of Cs [20]. This allows us to improve the accuracy in the determination of β, and thus in the interpretation of the PNC measurements, by incorporating the experimental results into our calculations.

The calculations were done using direct summation over the exact intermediate states,

$$\beta=\frac{e^2}{9}\sum_n \Bigg[\langle 7s|r|np_{1/2}\rangle\langle np_{1/2}|r|6s\rangle \times\left(\frac{1}{E_{7s}-E_{np_{1/2}}}-\frac{1}{E_{6s}-E_{np_{1/2}}}\right) -\langle 7s|r|np_{3/2}\rangle\langle np_{3/2}|r|6s\rangle \times\left(\frac{1}{E_{7s}-E_{np_{3/2}}}-\frac{1}{E_{6s}-E_{np_{3/2}}}\right)\Bigg]. \tag{3}$$

Here $\langle s|r|np\rangle$ is an effective radial integral for electromagnetic transitions between exact atomic eigenstates, which are related to the reduced matrix elements by

$$\langle s||r||p_{1/2}\rangle=\langle p_{1/2}||r||s\rangle=\sqrt{\tfrac{2}{3}}\langle s|r|p_{1/2}\rangle, \tag{4}$$

$$\langle s||r||p_{3/2}\rangle=-\langle p_{3/2}||r||s\rangle=\sqrt{\tfrac{4}{3}}\langle s|r|p_{3/2}\rangle. \tag{5}$$

It easy to see that β vanishes in the absence of the spin-orbit interaction, which splits energy levels and radial integrals. Thus, it is practically impossible to do accurate calculations of β using experimental results due to the strong cancelation between different terms, which causes the relative statistical error to be larger. Therefore, we calculated the scalar transition polarizability α instead and used the measured ratio α/β to find β. Note however, that the calculation of α/β using theoretical radial integrals and experimental energies reproduces the experimental value for this ratio with an accuracy of about 1%.

The expression for α is given by

$$\alpha=\frac{e^2}{9}\sum_n \Bigg[\langle 7s|r|np_{1/2}\rangle\langle np_{1/2}|r|6s\rangle \times\left(\frac{1}{E_{7s}-E_{np_{1/2}}}+\frac{1}{E_{6s}-E_{np_{1/2}}}\right) +2\langle 7s|r|np_{3/2}\rangle\langle np_{3/2}|r|6s\rangle \times\left(\frac{1}{E_{7s}-E_{np_{3/2}}}+\frac{1}{E_{6s}-E_{np_{3/2}}}\right)\Bigg]. \tag{6}$$

Here all of the major terms produce positive contributions. This reduces the error in the final result. 98% of the value of α is given by the intermediate $6p$ and $7p$ states. The $6p$ state does not contribute to the error in the final result. Our calculations of the $6s-6p$ electromagnetic amplitudes were recently confirmed with an accuracy of about 0.1% by very accurate experimental measurements [21]. The $6p$-$7s$ amplitudes are also known from [21] to have an accuracy of 0.5% and they agree with the theory.

The main source of error is the contribution of the $7p$ intermediate state. The radial integrals $\langle 6s|r|7p_{1/2}\rangle$ and $\langle 6s|r|7p_{3/2}\rangle$ are anomalously small due to cancelations between different areas of the integration in the single-particle amplitudes. These cancelations substantially increase the relative error in the calculated results. Because of this we use the experimental values of the $6s$-$7p$ transition amplitudes, which have an accuracy of about 0.7% [22]. In [22] the relative oscillator strengths were measured using the lifetime of the $6p_{1/2}$ state measured in [23] as a normalization point. Recent measurements of the lifetime are more accurate [20]. Therefore, we rescaled the experimental $6s$-$7p$ amplitudes from [22], using the new normalization. Note that the difference between $\langle 6s|r|7p_{1/2}\rangle$ and $\langle 6s|r|7p_{3/2}\rangle$ can be calculated very accurately. This is because it is proportional to the mixing between $7p$ and $6p$ states by the spin-orbit interaction. Indeed, perturbation theory in the spin-orbit interaction ξ gives

$$\langle 6s|r|7p_{1/2}\rangle-\langle 6s|r|7p_{3/2}\rangle\sim\frac{\xi_{7p6p}}{E_{7p}-E_{6p}}\langle 6s|r|6p\rangle+\cdots. \tag{7}$$

The values of the energy levels and spin-orbit splitting can be reproduced almost exactly in the numerical calculations by introducing factors into the correlation potential Σ (since the accuracy of the *ab initio* calculations is high, these factors are close to 1 anyway). The calculated matrix element $\langle 6s|r|6p\rangle$ practically coincides with the value obtained from the accurate measurements of Ref. [20]. Therefore, we believe that the absolute accuracy in the calculation of the difference between the doublet radial integrals is always higher than the experimental accuracy (to avoid confusion we should note that we use Dirac wave functions, i.e., we do not expand in ξ while doing calculations). Thus we can take the experimental value of $\langle 6s|r|7p_{1/2}\rangle$, which is measured more accurately, and find $\langle 6s|r|7p_{3/2}\rangle$, using the calculated difference $\langle 6s|r|7p_{3/2}\rangle-\langle 6s|r|7p_{1/2}\rangle$. Surprisingly, the result of this procedure gives precisely the result of the measurement of the $\langle 6s|r|7p_{3/2}\rangle$ amplitude, which formally has a larger error (1.8%). The ratio $\langle 6s|r|7p_{3/2}\rangle/\langle 6s|r|7p_{1/2}\rangle$ also has a

TABLE I. Radial integrals used in the calculation of α.

np	$\langle 6s\|r\|np\rangle$	$\langle np\|r\|7s\rangle$
$6p_{1/2}$	−5.5091(75)	5.190(27)
$6p_{3/2}$	−5.4824(62)	5.605(27)
$\Delta(6p_{3/2}-6p_{1/2})$	0.0267	0.4154
$7p_{1/2}$	−0.3460(26)	−12.597(38)
$7p_{3/2}$	−0.5040(38)	−12.372(37)
$\Delta(7p_{3/2}-7p_{1/2})$	−0.158	0.225

smaller experimental error (0.4%) than the error in $\langle 6s|r|7p_{3/2}\rangle$ [22]. Therefore, we may assume that the actual relative error in the $\langle 6s|r|7p_{3/2}\rangle$ is 0.7%, similar to that in $\langle 6s|r|7p_{1/2}\rangle$. We use theoretical values of the $\langle 7s|r|7p\rangle$ transition amplitudes since we believe that the expected theoretical error here (0.3%) is smaller than the experimental error. All higher transitions, including continuum and core electron transitions, were also calculated theoretically, even though their contribution was small (see below).

The result of the calculation of α is as follows:

$$\begin{aligned}\alpha &= \alpha(6p_{1/2})+\alpha(6p_{3/2})+\alpha(7p_{1/2})+\alpha(7p_{3/2})+\alpha(\text{others})\\ &= -32.39(0.17)-92.56(0.46)-(37.79+103.01)(1.14)\\ &\quad -3.25(0.20)=-269.0(1.3).\end{aligned} \tag{8}$$

We used experimental energy levels from [24] and radial integrals from Table I to calculate the contributions of the $6p$ and $7p$ states. We used both experimental and theoretical data to select the ''best values'' of these integrals. Note that the errors in $\alpha(7p_{1/2})$ and $\alpha(7p_{3/2})$ are proportional and so we added them. When new data for electromagnetic amplitudes are available it will be easy to refine this result by multiplying the corresponding term by the ratio of the new amplitude to the old one.

This value of α combined with the measurements of α/β [19] gives

$$\beta = 27.15(13)a_0^3. \tag{9}$$

The result of the direct calculation using radial integrals from Table I is $\beta=27.00$. The results of other works are $\beta=27.0(2)$ [17], $\beta=27.2(4)$ [25], $\beta=27.3(4)$ [26], and $\beta=27.17(35)$ [27]. Using Eq. (9), the measurement (1), the mean value of the theoretical amplitudes (2), and $|e|/a_0^2=5.1422\times10^{12}$ mV/cm, we obtain

$$Q_W(\text{expt}) = -72.41(25)_{expt}(80)_{theor}. \tag{10}$$

Comparing this result for Q_W with the theoretical value [28]

$$Q_W(\text{theor}) = -73.20(13)-0.8S-0.005T, \tag{11}$$

we can find the Peskin-Takeuchi parameter S characterizing new physics beyond the standard model (i.e., weak isospin conserving radiative corrections produced by new particles)

$$S+0.006T = -1.0(0.3)_{expt}(1.0)_{theor}. \tag{12}$$

We can also use the calculation of the extra Z_x-boson contribution in the SO(10) model [28]

$$\Delta Q_W = 0.4(2N+Z)\left(\frac{M_W}{M_{Z_x}}\right)^2 = 84.4\left(\frac{M_W}{M_{Z_x}}\right)^2, \tag{13}$$

to find the limit for the mass of this boson

$$M_{Z_x} > 550 \text{ GeV}. \tag{14}$$

The natural question is: can we refine the value of the E_{PNC} calculation using experimental $E1$ amplitudes? Unfortunately, the experimental accuracy at the moment is not good enough to make an improvement. For example, we can use the results of the work [17], where the direct sum-over-states approach was discussed in detail. The theoretical result of the direct summation was

$$E_{PNC} = -0.907(9)10^{-11}i|e|a_0\left(-\frac{Q_W}{N}\right). \tag{15}$$

Replacing the $E1$ amplitudes calculated in [17] (see Table IV of that work) with the values from Table I gives

$$E_{PNC} = -0.902(11)_{E1}(\sim 7)_{other}10^{-11}i|e|a_0\left(-\frac{Q_W}{N}\right). \tag{16}$$

Here we separated the error coming from the $6p$ and $7p$ $E1$ amplitudes from the error coming from all other sources, including the weak matrix elements and the amplitudes for transitions to the states above $7p$. The error in the weak matrix elements can be roughly estimated using the deviation of the calculated hyperfine intervals from the experimental values since both the weak and hyperfine interactions are approximately proportional to the density of the electron wave function near the nucleus. Note that the error from the $E1$ amplitudes exceeds the error in the theoretical values for the E_{PNC} (2). To avoid confusion we should stress that the calculation in Ref. [6] was based on the Green's-function technique and does not contain partial cancellations of the different terms that increase the error in the direct sum-over-state approach.

In conclusion, we would like to stress that accurate measurements of the $E1$ amplitudes (Table I) are very desirable for an improvement of the interpretation of the PNC measurements in Cs. For α the most important improvement would be a more accurate value of the $6s$-$7p$ amplitude. An improvement for the $7s$-$7p$ amplitude is also very important because of the disagreement between theory and existing data.

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