

High-Accuracy Calculation of the $6s_{1/2} \rightarrow 7s_{1/2}$ Parity-Nonconserving Transition in Atomic Cesium and Implications for the Standard Model

S. A. Blundell, W. R. Johnson, and J. Sapirstein

University of Notre Dame, Notre Dame, Indiana 46556

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A many-body calculation of the parity-nonconserving amplitude for the $6s_{1/2} \rightarrow 7s_{1/2}$ transition in atomic cesium with an error of order 1% is presented, $E_{\text{PNC}} = -0.906[9](Q_W/-N)i|e|a_0 \times 10^{-11}$. Using this result to determine Q_W from high-precision measurements of the transition leads to a quantitative test of the standard model. The various sources contributing to this transition are discussed and their uncertainties estimated. A discussion of radiative corrections with emphasis on the role of the top-quark mass is given.

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The recent accurate determination¹ of the mass of the Z has ushered in a new phase of the study of the weak interactions, that of high-precision tests of the theory which are sensitive to radiative corrections, the finiteness of which was a prime motivation for the introduction of unified theories of weak and electromagnetic interactions.² To study radiative corrections to the standard model, it is desirable to have as many highly accurate tests of the theory as possible. One such test is provided by the measurement of the parity-nonconserving (PNC) $6s_{1/2} \rightarrow 7s_{1/2}$ transition in atomic cesium.³ Observations of PNC transitions have been made in a number of atoms,⁴ but we concentrate here on atomic cesium because there have been advances in both theory⁵⁻⁹ and experiment^{10,11} that have the potential of changing the qualitative test of neutral currents so far provided by atomic PNC to a quantitative test, second in accuracy only to the Z mass measurement as a determination of θ_W . To gain quantitative information about the standard model from atomic PNC, it is clearly important to review carefully the various sources of the effect and the uncertainties associated with each, which is done in Secs. (1)–(4) below. Once these issues are discussed, we are in a position to show how a high-accuracy measurement of PNC transitions in cesium can be interpreted to give information about θ_W and the behavior of radiative corrections in the standard model.

The dominant effect that induces PNC transitions between the $6s_{1/2}$ and $7s_{1/2}$ states in cesium is described by the weak Hamiltonian

$$H_W = (G_F/\sqrt{8})Q_W\rho_{\text{nuc}}(r)\gamma_5, \quad (1)$$

where $\rho_{\text{nuc}}(r)$ is a combination of the neutron and proton densities in the cesium nucleus discussed further below and the weak charge Q_W is defined as

$$Q_W = 2[(2Z + N)C_{1u} + (Z + 2N)C_{1d}], \quad (2)$$

where C_{1u} and C_{1d} are the vector couplings of up and down quarks to the neutral current. It is important to emphasize at this point that atomic PNC measurements are uniquely sensitive to this combination of C_{1u} and

C_{1d} , and thus even with precision of a few percent, provide some of the most stringent limits to modifications of the standard model involving extra Z bosons.¹² To justify the use of this Hamiltonian one starts with the current-current interaction induced by the exchange of a Z between an electron and the nucleus, which leads to PNC transitions when the electron current is axial vector and the nuclear current vector (A_e, V_N) or vice versa (V_e, A_N). H_W is associated with the time component of (A_e, V_N); the space component of (A_e, V_N) and both the time and space components of (V_e, A_N) are relatively small and will be discussed under heading (3). Because it is the fourth component of a conserved vector current, the nuclear matrix element is not renormalized by the strong interactions, and is directly proportional to a weighted average of the number density of up and down quarks in the nucleus, which in turn depends on the neutron and proton distributions in the nucleus. The uncertainties associated with these distributions will be discussed under heading (2).

(1) The effect of H_W is to give each state of the atom a very small opposite-parity admixture, so that $s_{1/2}$ states contain some $p_{1/2}$ components, which gives the normally magnetic dipole ($M1$) transition $6s_{1/2} \rightarrow 7s_{1/2}$ a small electric dipole ($E1$) component. A powerful and systematic approach to calculating the $E1$ matrix element is the use of various methods of many-body perturbation theory (MBPT), which have been applied extensively to cesium by several groups.⁵⁻⁷ In the present work we have obtained agreement between two different MBPT schemes. In the first we saturate the sum over intermediate many-body states $|i\rangle$ in the expression

$$E_{\text{PNC}} = \sum_i \left[\frac{\langle 7s | H_W | i \rangle \langle i | D | 6s \rangle}{\epsilon_{7s} - \epsilon_i} + \frac{\langle 7s | D | i \rangle \langle i | H_W | 6s \rangle}{\epsilon_{6s} - \epsilon_i} \right]. \quad (3)$$

We have developed a technique¹³ which sums certain infinite classes of MBPT diagrams, allowing calculations of hyperfine constants in Cs to be carried out at the 1% level of accuracy, and calculations of energies and allowed $E1$ matrix elements to 0.5% or better. By includ-

ing the $|i\rangle = |6p_{1/2}\rangle, |7p_{1/2}\rangle, |8p_{1/2}\rangle,$ and $|9p_{1/2}\rangle$ atomic states explicitly in Eq. (3) with this technique, and then estimating the omitted contributions (which amount to about 2%) using low orders of MBPT, we find for E_{PNC} and the vector Stark polarizability β for the $6s_{1/2}$ - $7s_{1/2}$ transition

$$E_{\text{PNC}}(\text{theory}) = -0.906[9](Q_W/N)i|e|a_0 \times 10^{-11}, \quad (4a)$$

$$\beta(\text{theory}) = 27.00[20]a_0^3. \quad (4b)$$

Note that we adopt a convention of using square brackets for theoretical uncertainties and parentheses for experimental error. The coefficient -0.906 in E_{PNC} includes a Breit correction of 0.002, which is found by adding the Breit to the Coulomb interaction everywhere in a Dirac-Fock level calculation. The calculation of β is similar to that of E_{PNC} , with H_W essentially replaced by a second dipole operator D . The theoretical errors quoted here are based on the following tests: (a) We modify the wave functions slightly to fit energies; (b) we make similar modifications to fit instead hyperfine constants; (c) we compare the dipole operator in both its length and velocity forms; and (d) we use experimentally available energies and oscillator strengths where possible instead of the calculated ones. The resultant scatter in values of E_{PNC} and β is used to determine the errors. The error estimates represent the largest changes in E_{PNC} and β generated by the modifications described above.

In our second method we include the effect of H_W in the single-particle states, which acquire opposite-parity admixtures; we then use these parity-mixed states in a MBPT calculation of a dipole matrix element. Specifically, we solve for normalized quasiparticle orbitals φ_i for the $6s_{1/2}$ and $7s_{1/2}$ states which satisfy

$$(h_{\text{DF}} + \Sigma^{(2)})\varphi_i = \varepsilon_i \varphi_i. \quad (5)$$

Here $\Sigma^{(2)}$ is the second-order self-energy operator, and h_{DF} is the Dirac-Fock (DF) Hamiltonian. The solution of (5) is equivalent to summing an infinite sequence of chains of $\Sigma^{(2)}$. Each state φ_i acquires an opposite-parity admixture $\tilde{\varphi}_i$ which we calculate by adding H_W to h_{DF} in the core DF equations and in Eq. (5), and by linearizing the resulting equations in H_W . Finally, we evaluate

$$E_{\text{PNC}} = \langle \tilde{\varphi}_{7s} | (D + D_{\text{RPA}}) | \varphi_{6s} \rangle + \langle \varphi_{7s} | (D + D_{\text{RPA}}) | \tilde{\varphi}_{6s} \rangle + \langle \varphi_{7s} | \tilde{D}_{\text{RPA}} | \varphi_{6s} \rangle + E_{\text{SR}} + E_{\Sigma} + E_{\text{norm}}, \quad (6)$$

where D_{RPA} is the RPA modification to the dipole operator, and the last three terms are small contributions from structural radiation,¹³ internal opposite-parity substitutions in $\Sigma^{(2)}$, and normalization, respectively. Because $\Sigma^{(2)}$ is a rather inaccurate approximation to the exact self-energy, we repeat the calculation with $\Sigma^{(2)}$ replaced by $\lambda\Sigma^{(2)}$, where $\lambda=0.80$ for $s_{1/2}$ states and $\lambda=0.84$ for $p_{1/2}$ states were chosen to fit energies. The prediction for

E_{PNC} changes by only a few tenths of a percent. This calculation agrees with the result of the previous very different approach to within our quoted error on E_{PNC} .

The most complete alternative calculation of E_{PNC} in the literature is by members of the Novosibirsk group,⁵ who obtain a coefficient $-0.91[1]$, in good agreement with our value. Our second calculational scheme follows closely the approach they introduced, except that they calculate explicitly an infinite subset of higher-order corrections to the self-energy operator, rather than rely on a scaling parameter λ as we did. There is close agreement between the individual contributions in their calculation and the present one.

In an earlier calculation which treated $\Sigma^{(2)}$ only in leading order,⁶ we obtained a coefficient $-0.951[50]$. Hartley, Lindroth, and Martensson-Pendrill have recently performed a similar calculation,⁷ confirming our earlier result, and including an additional cross term between the RPA correction and the self-energy operator, leading to a value $-0.936[37]$. This cross term is also included in the present calculation and in the calculation of the Novosibirsk group. The primary reason for the disagreement with our present result is that we chain the self-energy by solving the full quasiparticle equation (5), which accounts for a further -3% reduction.

We mention also the semiempirical results $-0.935(19)[28]$ (Ref. 8) and $-0.904[18]$ (Ref. 9). While all calculations are consistent within quoted errors, it is still a major challenge to atomic theory to provide even more accurate results as the precision of the experiments improves.

(2) The charge density of the cesium nucleus has been determined by a muonic x-ray experiment:¹⁴ In terms of a spherical Fermi distribution it is given by

$$\rho_{\text{proton}}(r) = \rho_0 [1 + e^{-(r-c)/a}]^{-1}, \quad (7)$$

with $a=2.3/4(\ln 3)$ fm and $c=5.6743(10)$ fm. Unfortunately, the neutron density, which enters significantly into the weak Hamiltonian, is not experimentally available. We have used a theoretical determination¹⁵ of this density based on a theory that reproduces the charge radius, and gives for the neutron distribution

$$\rho_{\text{neutron}}(r) = \rho'_0 [1 + e^{-(r-c')/a'}]^{-b}, \quad (8)$$

with $c'=6.153$ fm, $a'=0.64823$ fm, and $b=1.589$. When an appropriately weighted neutron and proton distribution was used in place of the charge distribution, the lowest-order Dirac-Fock result changed by only 0.08%. While there is, of course, some theoretical uncertainty in the determination of this distribution, the relative insensitivity of atomic PNC makes this error entirely negligible compared to the theoretical uncertainty discussed under heading (1).

(3) H_W , as discussed above, comes from the time component of (A_e, V_N) . The spatial component of this term and the time component of (V_e, A_N) are highly sup-

pressed: We estimate their size at under 0.1%. Turning to the spatial part of the latter term, it can be shown that its effect is described by the Hamiltonian

$$H_W^{(2)} = -\frac{G_F}{\sqrt{2}} K_2 \frac{\kappa - \frac{1}{2}}{I(I+1)} \mathbf{a} \cdot \mathbf{I} \rho(r), \quad (9)$$

where $\kappa=4$ for the unpaired proton of ^{133}Cs and $K_2 \approx -0.05$. In addition, the existence of parity violation within the nucleus leads to a parity-violating magnetic moment called the anapole moment,¹⁶ that leads to a Hamiltonian with a very similar structure,

$$H_W^{(a)} = \frac{G_F}{\sqrt{2}} K_a \frac{\kappa}{I(I+1)} \mathbf{a} \cdot \mathbf{I} \rho(r). \quad (10)$$

We treat Eqs. (9) and (10) together by replacing K_a with $K \equiv K_a - (\kappa - \frac{1}{2})/\kappa K_2$ in Eq. (10). While the nuclear distributions could be different, we have found little sensitivity to the details of the distribution; results from a Fermi distribution differ from a crude shell-model calculation distribution by less than 2%. Because both of these effects are sensitive to questions of nuclear structure and strong-interaction corrections, the uncertainties of such calculations could be a serious problem for interpretation of atomic PNC. However, experiments measure different hyperfine transitions, and it is possible to eliminate the effect of both $H_W^{(2)}$ and $H_W^{(a)}$ by taking appropriate linear combinations of the different measurements. Specifically, the spin- $\frac{7}{2}$ nucleus couples to the electron $s_{1/2}$ states to form multiplets with total spin $F=3$ and 4. The contributions to the PNC amplitude from $H_W^{(a)}$ and $H_W^{(2)}$ calculated in the Dirac-Fock approximation, including weak core-polarization corrections, lead to the following spin-dependent result for $6s_{1/2}(F) \rightarrow 7s_{1/2}(F')$:

$$E_{\text{PNC}} = -0.906[9] \left[\left[\frac{Q_W}{-N} \right] + A(F', F) K \right] \times i |e| a_0 \times 10^{-11}, \quad (11)$$

with $A(3,3)=0.029$, $A(4,3)=-0.041$, $A(3,4)=0.048$, and $A(4,4)=-0.022$. The values of the coefficients $A(F', F)$ agree to within 10% with results from semi-empirical¹⁷ and MBPT¹⁸ calculations. Thus, as will be discussed below, appropriate linear combinations can either isolate nuclear-spin-dependent effects, or, if one is interested in testing the standard model with the least possible theoretical uncertainty, eliminate them.

(4) Finally, we consider the effect of Z exchange between two electrons. This is described by the Hamiltonian

$$H_W^{(3)} = -\frac{G_F}{\sqrt{32}} (1 - 4 \sin^2 \theta_W) \times \sum_{i \neq j} (\gamma_3^i + \gamma_3^j) (1 - \mathbf{a}_i \cdot \mathbf{a}_j) \delta^3(r_i - r_j). \quad (12)$$

We have calculated the lowest-order contribution to

E_{PNC} from this Hamiltonian in the DF approximation, and find that it contributes under 0.1% of the basic term, and can be neglected at the present level of accuracy.

Once the precision of atomic PNC is at the 1% level, it is necessary to include radiative corrections properly. While at tree level Q_W depends only on θ_W , radiative corrections depend on two unknown quantities, the mass of the Higgs boson m_H , and the mass of the top quark m_t . Because θ_W must be inferred from experiment using radiative corrections, its value thus depends on m_H and m_t . However, the dependence of θ_W on m_H is quite weak, and in a particular renormalization scheme, the modified minimal-subtraction scheme,¹⁹ the dependence of θ_W on m_t is also relatively weak. The most recent determination of θ_W in the modified minimal-subtraction scheme, using the precise Z mass measurement¹ and assuming $m_H = 100$ GeV, is²⁰

$$\sin^2 \hat{\theta}_W(m_W) = \begin{cases} 0.2328(5), & m_t = 100 \text{ GeV}, \\ 0.2301(4), & m_t = 200 \text{ GeV}. \end{cases} \quad (13)$$

Considering now only the standard model we introduce the one-loop radiatively corrected form

$$Q_W = \rho' \{ -N + Z [1 - 4\kappa' \sin^2 \hat{\theta}_W(m_W)] \} \approx [0.9796 + 0.0020 m_t^2 / m_W^2] \times \{ -N + Z [1 - 4.012 \sin^2 \hat{\theta}_W(m_W)] \}. \quad (14)$$

This equation is an approximation to the relatively complex formulas for ρ' and κ' given in Ref. 19. We are now in a position to extract information from a high-accuracy measurement of cesium PNC. The most accurate experiment¹¹ reports

$$\text{Im}(E_{\text{PNC}})/\beta = \begin{cases} -1.513(50) \text{ mV/cm} & (F=3 \rightarrow F'=4), \\ -1.639(48) \text{ mV/cm} & (F=4 \rightarrow F'=3). \end{cases} \quad (15)$$

Using Eq. (11) we can either extract a value of E_{PNC} independent of $H_W^{(a)}$ and $H_W^{(2)}$, or alternatively determine $K=0.83(46)$, which is consistent with the theoretical estimates²¹ $K=0.29-0.37$. The former procedure, which is close to taking an average of the two transitions, leads to $\text{Im}(E_{\text{PNC}})/\beta = -1.572(35)$ mV/cm. Using the value of β from Eq. (4b) and converting into the units of Eq. (4a) gives the experimental value

$$E_{\text{PNC}}^{(\text{exp})} = -0.8252(184)[61] i |e| a_0 \times 10^{-11}. \quad (16)$$

Then using Eq. 4(a) we can finally determine Q_W as

$$Q_W = -71.04(1.58)[0.88], \quad (17)$$

where we have taken the two theoretical errors in quadrature.

We can now comment on the implications for the standard model of atomic PNC. When m_t is much smaller than m_W , the dependence of ρ' on this parameter is negligible. However, because the lower limit of m_t is

significantly larger than the value 45 GeV used in earlier works,¹² one must specify a value for it before a determination of θ_W can be made. In the following we treat two cases, $m_t = 100$ and 200 GeV. We find

$$\sin^2 \hat{\theta}_W(m_W) = \begin{cases} 0.2242(65)[36], & m_t = 100 \text{ GeV}, \\ 0.2215(65)[36], & m_t = 200 \text{ GeV}. \end{cases} \quad (18)$$

It is of interest to note that, if the experimental error can be reduced to below the theoretical error, this method of determining θ_W will compete in accuracy with neutrino scattering.¹²

The 1.2% variation in the central value of $\sin^2 \hat{\theta}_W(m_W)$ in Eq. (18) as m_t varies from 100 to 200 GeV would appear to present a barrier to accurate tests of the standard model while m_t is still unknown. The same problem occurs for the Z mass determination of $\sin^2 \hat{\theta}_W(m_W)$, as can be seen from the 1.2% variation in Eq. (13). However, the dependence on m_t is almost identical, and so if one takes $\sin^2 \hat{\theta}_W(m_W)$ from Eq. (13) and applies it in Eq. (14), the resulting value $Q_W = -73.1$ is essentially independent of m_t . For this reason atomic PNC taken together with the Z mass determination cannot give information about the top-quark mass, but instead allows a test of radiative corrections to the standard model and a probe sensitive to new physics free of the uncertainty caused by the unknown value of m_t .

To repeat the main conclusion of this Letter, the theoretical status of atomic PNC has improved to a point where the next generation of experiments will provide quantitative constraints on the standard model. Atomic PNC is insensitive to m_t when the mass of the Z is used to determine θ_W , so that an unambiguous test is allowed by a high-accuracy experiment. We have examined several sources of theoretical error, and have found that the dominant error is still associated with the calculation of E_{PNC} and β . The reduction of this error to the tenth of a percent level is an outstanding challenge to many-body theory. However, even at the 1% level, atomic PNC has a significant role to play as one of a set of ever more precise experimental tests of the standard model.

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