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### Correlation effects in the parity-nonconserving $6s \rightarrow 7s$ transition in cesium

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The amplitude of the parity-nonconserving (PNC) electric-dipole transition  $6s \rightarrow 7s$  in cesium is calculated to third order in many-body perturbation theory. Inclusion of the corresponding corrections in calculations of parity-conserving transition amplitudes and atomic hyperfine constants leads to agreement with experiment at a level under 5%. We obtain a value of  $0.951iea_0 \times 10^{-11} Q_W / -N$  with an estimated error of 5% for the PNC amplitude. A determination of the Weinberg angle is made by combining the present calculation with recent measurements of the PNC amplitude: the result is  $\sin^2 \theta_W = 0.229(24)_{\text{expt}}(16)_{\text{theor}}$ . Issues involved in improving the accuracy of the calculations of atomic properties of cesium are discussed.

While the Weinberg-Salam model<sup>1</sup> is an extremely successful theory of weak interactions, most of its predictions can be obtained from the tree-level structure of the theory. Since one of the most important features of the model is its renormalizability, precision comparisons between theory and experiment are necessary if the loop structure of the theory is to be rigorously tested. In particular, the relatively poorly understood Higgs sector can be probed in this manner because if the Higgs boson is truly a fundamental scalar, it enters into loop calculations in a well-defined manner. Therefore precision studies of weak-interaction processes offer a way of probing the structure of symmetry breaking using available laboratory facilities which complements tests seeking to explore this structure by, say, directly producing either the Higgs boson or else uncovering new physics associated with a more fundamental understanding of the Higgs mechanism.

A direct test of radiative corrections is provided simply by measuring the masses of the  $W$  and  $Z_0$  bosons. Provided that the Weinberg angle  $\theta_W$  is known, and given the accurately determined Fermi and fine-structure constants, any deviations from the tree-level prediction

$$M_W^2 = \frac{\pi\alpha}{2G_W \sin^2 \theta_W}, \quad M_Z = \frac{M_W}{\cos \theta_W},$$

must be attributed to these radiative corrections. However, without an independent measurement of  $\theta_W$ , while still possible, it is more difficult to extract such information from the  $W$  and  $Z_0$  masses. The status of radiative corrections has been discussed in a recent paper by Amaldi *et al.*<sup>2</sup> The strongest tests of these corrections are shown in that paper to arise not from a study of the

weak-boson masses in isolation, but rather from considering a variety of weak-interaction processes together. Among such processes are parity-nonconserving (PNC) electric-dipole transitions in atomic systems, which for heavy atoms are sensitive to the weak charge,  $Q_W$ , defined as

$$Q_W = Z(1 - 4 \sin^2 \theta_W) - N, \quad (1)$$

where  $N$  is the number of neutrons in the nucleus and  $Z$  the atomic number. This quantity is modified by radiative corrections,<sup>3</sup> and will be further discussed when comparison with experiment is made. While the theory of PNC transitions in hydrogen<sup>4</sup> is well understood, PNC effects have not been detected in this atom despite vigorous efforts. However, PNC effects have been clearly seen in heavy atoms. The most accurate published measurements of PNC amplitudes are for the  $6s \rightarrow 7s$  transition in cesium;<sup>5,6</sup> these measurements are accurate at roughly the 10% level. A measurement of the PNC  $6p_{1/2} \rightarrow 7p_{1/2}$  amplitude in thallium accurate to 15% has also been made.<sup>7</sup> In order to extract values of  $Q_W$  from these measurements in heavy atoms, it is necessary that the complex atomic structure of the atoms be understood to at least the experimental level of accuracy. It is this problem of determining accurate theoretical PNC amplitudes that we address in the present paper. Because cesium is an alkali-metal atom, the atomic structure problems are less severe than for thallium or for the other heavy atoms in which parity nonconservation has been observed, namely Pb (Ref. 8) and Bi (Ref. 9). We therefore restrict our attention to cesium and do not treat these other interesting systems here.

A large amount of theoretical effort has gone into pre-

dicting the strength of PNC amplitudes in Cs: a review of this work has been given by Mårtensson-Pendrill.<sup>10</sup> There have been a variety of potential model calculations, including a recent calculation that combines the use of empirical data with many-body perturbation theory (MBPT),<sup>11</sup> and also a number of Hartree-Fock (HF) calculations (we start our calculations using a HF potential). The lowest-order Hartree-Fock value is well established to be  $0.927iea_0 \times 10^{-11} Q_W / -N$ . MBPT corrections at the next order associated with the random-phase approximation (RPA) have been calculated by several groups,<sup>12-14</sup> and good agreement between the different calculations has been found. Inclusion of the RPA effects reduces the PNC amplitude to  $0.890iea_0 \times 10^{-11} Q_W / -N$ .

It has been shown recently<sup>15</sup> that including a particular subset of the third-order correlation corrections, those associated with Brueckner orbitals, in calculations of transition amplitudes in alkali-metal atoms gives theoretical amplitudes which agree with precisely measured experimental amplitudes to within a few percent for the heavier alkali metals, rubidium and cesium. An essential feature of the work in Ref. 15 was the use of basis sets constructed from  $B$  splines and restricted to a cavity of finite but large radius.<sup>16</sup> Use of these basis sets allowed the infinite sums and continuum integrals of perturbation theory to be replaced by finite sums. It is entirely straightforward to extend the calculations of Ref. 15 to treat parity-nonconserving transitions since the effect is very small and can be reliably calculated by treating the weak interaction in first-order perturbation theory. To this end we replace the basis functions used in the calculation of parity-conserving amplitudes by parity-mixed basis functions. These parity-mixed basis functions are obtained by adding to each of the orbitals used in the calculations of parity-conserving amplitudes the first-order correction of the opposite parity induced by the weak interaction. To determine the (Coulomb field) correlation corrections to the PNC amplitude we simply linearize in the weak interaction the expressions for the correlation corrections to the parity-conserving amplitude. For example, to obtain the correlation correction to the parity-forbidden electric-dipole amplitude for  $v \rightarrow w$ , where  $v$  and  $w$  are valence states of the same parity, from a term in second-order perturbation theory such as

$$Z^{(2)} = \sum_{n,a} \frac{z_{an} g_{wnva}}{\epsilon_a + \epsilon_v - \epsilon_n - \epsilon_w} \quad (2)$$

we simply evaluate

$$\begin{aligned} Z_{\text{PNC}}^{(2)} = & \sum_{n,a} \frac{z_{an} g_{wnva}}{\epsilon_a + \epsilon_v - \epsilon_n - \epsilon_w} + \sum_{n,a} \frac{z_{an} g_{wnva}}{\epsilon_a + \epsilon_v - \epsilon_n - \epsilon_w} \\ & + \sum_{n,a} \frac{z_{an} g_{\bar{w}nva}}{\epsilon_a + \epsilon_v - \epsilon_n - \epsilon_w} + \sum_{n,a} \frac{z_{an} g_{\bar{w}nva}}{\epsilon_a + \epsilon_v - \epsilon_n - \epsilon_w} \\ & + \sum_{n,a} \frac{z_{an} g_{wn\bar{v}a}}{\epsilon_a + \epsilon_v - \epsilon_n - \epsilon_w} + \sum_{n,a} \frac{z_{an} g_{wn\bar{v}a}}{\epsilon_a + \epsilon_v - \epsilon_n - \epsilon_w}, \end{aligned} \quad (3)$$

where the parity-nonconserving correction  $|\bar{i}\rangle$  to the

state  $|i\rangle$  satisfies

$$(H_{\text{HF}} - \epsilon_i) |\bar{i}\rangle = -(h_W + V_{\text{PNC}}) |i\rangle. \quad (4)$$

The notation used here is explained in more detail in Ref. 14. When expressed in terms of radial functions, minus signs in the first, third, and fourth terms of Eq. (3) are present because of an implicit factor of  $i$  in the definition of parity-nonconserving corrections, which requires that the complex conjugate of these states have the factor  $-i$ . The PNC counterparts to core states,  $|\bar{a}\rangle$ , are obtained from the recursive solution of Eq. (4) for a core state  $a$  using standard differential equation techniques, and then these functions are used to solve the equation for the entire basis set using spline techniques.

While it is in principle straightforward, the evaluation of the parity-nonconserving corrections  $|\bar{i}\rangle$  requires very careful treatment in the framework of the spline method. This added care is required since the weak interaction Hamiltonian  $h_W$  in Eq. (4) vanishes outside the nucleus, so that it is important to have highly accurate solutions for  $r$  smaller than the nuclear radius. To accomplish this using spline basis functions requires the use of a carefully chosen radial grid. We find that by placing 15 spline knots on a linear grid from  $r=0-0.00015$  a.u., followed by an exponential grid from  $0.00015$  a.u. to the cavity boundary, which was chosen to be  $45$  a.u., generates spline basis functions that agree precisely inside the nucleus with wave functions generated using standard differential equation techniques. It is, however, necessary to increase the number of basis functions from  $40$  (the number used in Ref. 15 for calculations of parity-conserving amplitudes in cesium) to  $60$ . We have plotted in Fig. 1 the large components of PNC corrections to the  $6s$  and  $7s$  radial wave functions obtained using  $B$  splines. The norm of these spline-generated wave functions differs from the norm of wave functions generated by solving the differential equations (4) by about  $50$  parts per million. The lowest-order PNC amplitude obtained using  $B$  splines was found to agree with that obtained by solving Eq. (4) with differential equation techniques to five significant figures.

Since the calculation of the correlation corrections to the PNC amplitude is quite complex it was coded independently in three different ways. In all three methods a subset of third-order MBPT corrections, the Brueckner-orbital contributions in Ref. 15, was evaluated. For parity-conserving transitions these corrections are given by

$$\begin{aligned} Z_{\text{BO}}^{(3)} = & \sum_{a,b,m,i} \left[ \frac{g_{abmv} z_{wi} (g_{miba} - g_{miab})}{(\epsilon_i - \epsilon_v)(\epsilon_v + \epsilon_m - \epsilon_a - \epsilon_b)} + \text{c.c.} \right] \\ & + \sum_{a,m,n,i} \left[ \frac{g_{aimn} z_{wi} (g_{mnav} - g_{mnva})}{(\epsilon_i - \epsilon_v)(\epsilon_n + \epsilon_m - \epsilon_a - \epsilon_v)} + \text{c.c.} \right], \end{aligned} \quad (5)$$

where c.c. means the operation of complex conjugation and the interchange of  $v$  and  $w$ . Here  $v$  and  $w$  denote different valence states ( $6s$  and  $7s$  for this calculation),  $a$  and  $b$  are core states,  $m$  and  $n$  excited states including valence states, and  $i$  all states. In the following the first

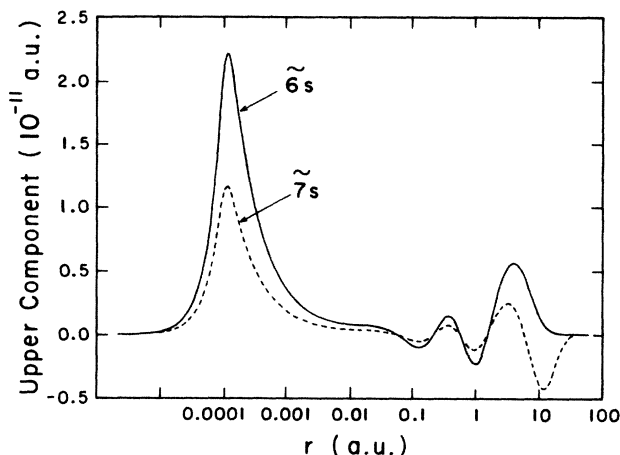


FIG. 1. The large components of the PNC corrections to the lowest-order  $6s$  and  $7s$  wave functions are plotted against  $r$  in atomic units.

term will be referred to as the single-excitation term because it involves a sum over one excited state, and the second will be called the double-excitation term. Implicit in both are partial wave summations: this summation is cut off at  $l = 6$  in the present calculation.

In all three methods we used an extension of the decomposition given in Eq. (3). In the first method, Eq. (5) was coded directly as nested loops. Since there are ten wave functions involved in each term, the PNC calculation consisted of evaluating each term ten times, with an opposite parity wave function inserted in each term.

Careful consideration must of course be given to the different angular momentum channels associated with changing the parity of the various wave functions. This direct method permits a determination of "internal" substitutions, in which the weak interaction acts on the internal lines of the Brueckner-Goldstone graphs associated with Eq. (5), as well as "external" substitutions, in which the weak interaction acts at the outside lines of the graph. Specifically, internal substitutions involve changing the parity of the states  $a$ ,  $b$ , or  $m$  for single excitations, and  $a$ ,  $m$ , or  $n$  for double excitations, while the external substitutions are obtained by changing the parity of  $v$ ,  $w$ , and  $i$ . The results for the external substitutions obtained using this method are presented in Table I, together with the contributions to the double-excitation part from the individual core states  $a$  in Eq. (5). Contributions from parts of the calculations in which the weak interaction perturbs the valence states or their Brueckner-orbital corrections are shown explicitly to exhibit strong cancellations between the different terms. These external contributions are combined with the corresponding contributions from internal substitutions in Table II to give the final Brueckner-orbital third-order correlation correction. It may be seen from these tables that external substitutions dominate internal substitutions in the final totals, although for individual core contributions this is not necessarily true.

The second and third approaches both exploit the fact that the correction  $Z_{BO}^{(3)}$  is associated with Brueckner orbitals. We define a lowest-order Brueckner-type modification to the valence orbital  $|v\rangle$  by

TABLE I. Contributions to the correlation corrections for the  $6s \rightarrow 7s$  amplitude in cesium from "external" substitutions. Notation:  $5p^* = 5p_{1/2}$ ,  $5p = 5p_{3/2}$ , etc. (Units:  $iea_0 \times 10^{-11} Q_W / -N$ .)

	$\langle 7s   r   \delta 6\bar{s} \rangle$	$\langle \delta 7s   r   6\bar{s} \rangle$	$\langle \delta 7\bar{s}   r   6s \rangle$	$\langle 7\bar{s}   r   \delta 6s \rangle$	Sum
	Single sums				
	-0.039 28	0.026 10	-0.010 99	0.050 94	0.026 78
	Double sums				
$5p$	0.145 55	-0.160 51	0.310 11	-0.288 83	0.006 32
$5p^*$	0.067 13	-0.070 17	0.127 12	-0.126 58	-0.002 50
$5s$	0.012 26	-0.013 89	0.031 70	-0.025 37	0.004 70
$4d$	0.027 92	-0.029 77	0.065 97	-0.055 58	0.008 54
$4d^*$	0.018 38	-0.019 36	0.042 13	-0.036 15	0.005 00
$4p$	0.003 64	-0.005 34	0.011 44	-0.007 72	0.002 02
$4p^*$	0.001 72	-0.001 85	0.004 37	-0.003 49	0.000 75
$4s$	0.000 74	-0.000 91	0.002 50	-0.001 71	0.000 62
$3d$	0.001 65	-0.002 36	0.007 54	-0.004 46	0.002 37
$3d^*$	0.001 09	-0.001 53	0.004 83	-0.002 89	0.001 49
$3p$	0.000 52	-0.000 71	0.002 20	-0.001 35	0.000 66
$3p^*$	0.000 25	-0.000 32	0.000 91	-0.000 60	0.000 25
$3s$	0.000 14	-0.000 20	0.000 63	-0.000 37	0.000 20
$2p$	0.000 13	-0.000 20	0.000 70	-0.000 38	0.000 24
$2p^*$	0.000 07	-0.000 10	0.000 30	-0.000 18	0.000 09
$2s$	0.000 03	-0.000 06	0.000 24	-0.000 12	0.000 09
$1s$	0.000 00	-0.000 03	0.000 13	-0.000 05	0.000 05
	0.241 94	-0.281 21	0.601 83	-0.504 89	0.057 67

TABLE II. External and internal correlation corrections to the PNC amplitude  $6s \rightarrow 7s$  in cesium. Notation:  $5p^* = 5p_{1/2}$ ,  $5p = 5p_{3/2}$ , etc. (Units:  $iea_0 \times 10^{-11} Q_W / -N$ .)

	External PNC	Internal PNC	Sum
	Single sums		
	0.026 78	-0.006 25	0.020 53
	Double sums		
5p	0.006 32	0.000 77	0.007 09
5p*	-0.002 50	0.009 35	0.006 85
5s	0.004 70	-0.003 88	0.000 82
4d	0.008 54	0.001 49	0.010 03
4d*	0.005 00	0.001 31	0.006 31
4p	0.002 02	-0.000 23	0.001 79
4p*	0.000 75	0.000 46	0.001 21
4s	0.000 62	-0.000 43	0.000 19
3d	0.002 37	0.000 22	0.002 59
3d*	0.001 49	0.000 17	0.001 66
3p	0.000 66	-0.000 05	0.000 61
3p*	0.000 25	0.000 21	0.000 46
3s	0.000 20	-0.000 19	0.000 01
2p	0.000 24	0.000 00	0.000 24
2p*	0.000 09	0.000 13	0.000 22
2s	0.000 09	-0.000 12	-0.000 03
1s	0.000 05	0.000 01	0.000 06
	0.057 67	0.002 97	0.060 64

$$|\delta v\rangle = \sum_{\substack{i,v \\ i \neq v}} \frac{|i\rangle\langle i| V_{\text{BO}} |v\rangle}{\epsilon_v - \epsilon_i}, \quad (6)$$

$$\langle i| V_{\text{BO}} |v\rangle = \sum_{a,b,m} \frac{(g_{abmv} - g_{bamv})g_{miba}}{\epsilon_a + \epsilon_b - \epsilon_v - \epsilon_m} + \sum_{a,m,n} \frac{(g_{mnva} - g_{mnva})g_{aimn}}{\epsilon_a + \epsilon_v - \epsilon_m - \epsilon_n}, \quad (7)$$

so that the sum  $|v\rangle + |\delta v\rangle$  gives an approximate Brueckner orbital correct to the lowest nonvanishing order of perturbation theory. In terms of these functions we may write  $Z_{\text{BO}}^{(3)}$  as

$$Z_{\text{BO}}^{(3)} = \langle \delta w | z | v \rangle + \langle w | z | \delta v \rangle. \quad (8)$$

In the second approach, we evaluate the Brueckner corrections with relativistic pair functions. Pair function techniques have been used extensively by Lindgren and co-workers,<sup>17</sup> and provide an elegant and powerful method of organizing MBPT. Although our method is based on finite basis sets, it is still possible to create the pair functions in lowest order by direct summation;

$$\rho_{ab}(\mathbf{r}_1, \mathbf{r}_2) = \sum_{m,n} \frac{g_{mnab}}{\epsilon_a + \epsilon_b - \epsilon_m - \epsilon_n} \psi_m(\mathbf{r}_1) \psi_n(\mathbf{r}_2). \quad (9)$$

In practice, however, we find it more convenient to work with the expansion coefficients of the pair function in the finite basis set:

$$\rho_{nmab} = \frac{g_{nmab}}{\epsilon_a + \epsilon_b - \epsilon_n - \epsilon_m}. \quad (10)$$

The Brueckner corrections can be evaluated in terms of one pair function and one  $g$  coefficient.

The parity-mixed version of these equations follows in the usual way. The Brueckner correction  $|\delta v\rangle$  has a PNC counterpart  $|\delta \bar{v}\rangle$  with the same  $j$  as  $|v\rangle$  but of the opposite parity. In addition, each pair function has a PNC counterpart,

$$\tilde{\rho}_{nmab} = \frac{g_{\bar{n}mab} + g_{n\bar{m}ab} + g_{nm\bar{a}b} + g_{nma\bar{b}}}{\epsilon_a + \epsilon_b - \epsilon_n - \epsilon_m}, \quad (11)$$

corresponding to a sum of  $g$  coefficients that always enters the equations in the above combination. The PNC Brueckner correction  $|\delta \bar{v}\rangle$  is given by

$$|\delta \bar{v}\rangle = \sum_{\substack{i,v \\ i \neq v}} \left[ \frac{|i\rangle\langle \tilde{i}| + |\tilde{i}\rangle\langle i|}{\epsilon_v - \epsilon_i} \right] V_{\text{BO}} |v\rangle + \sum_{\substack{i,v \\ i \neq v}} \frac{|i\rangle\langle i| V_{\text{BO}} |\bar{v}\rangle}{\epsilon_v - \epsilon_i} + \sum_{\substack{i,v \\ i \neq v}} \frac{|i\rangle\langle i| \tilde{V}_{\text{BO}} |v\rangle}{\epsilon_v - \epsilon_i}. \quad (12)$$

The third term on the right-hand side corresponds to the internal substitutions.

Formally these first two approaches are very similar; however, they lead to completely different organizations of the calculation, and this provides a valuable check against the possibility of computer coding errors in what are quite complex calculations. The pair function approach tends to be more efficient, although it places greater demands on computer memory and is somewhat more difficult to code.

The final calculation uses the fact that differential equation techniques allow for an evaluation of the external part of the calculation by solving the equation

$$(\epsilon_v - H_{\text{HF}}) |\delta \bar{v}\rangle_{\text{ext}} = (h_W + \tilde{V}_{\text{PNC}}) |\delta \bar{v}\rangle - \epsilon^{(2)} |\bar{v}\rangle + V_{\text{BO}} |\bar{v}\rangle, \quad (13)$$

where  $\epsilon^{(2)} \equiv \langle v | V_{\text{BO}} | v \rangle$ . Equation (13) is formally equivalent to Eq. (12) without the third term on the right-hand side.  $V_{\text{BO}}$  in Eq. (13) is still evaluated with splines, although the sums over  $|i\rangle$  and  $|\tilde{i}\rangle$  are performed with differential equation techniques. This approach provides a check on the completeness of the parity-mixed basis set  $|i\rangle + |\tilde{i}\rangle$ ; we obtain results that agree to three digits with the results for the external substitutions obtained from the other two approaches. We did not evaluate internal substitutions with the third method.

Adding the final correction from Table II,  $0.061iea_0 \times 10^{-11} Q_W / -N$ , to that previously obtained<sup>12-14</sup> at the level of the RPA,  $0.890iea_0 \times 10^{-11} Q_W / -N$ , we obtain the new result,  $0.951iea_0 \times 10^{-11} Q_W / -N$ . We can use this calculation to predict the strength of the PNC amplitude that should be seen in cesium. If we use the present world average for the Weinberg angle,<sup>2</sup>

$$\sin^2 \theta_W = 0.230(5), \quad (14)$$

$Q_W$  from Eq. (1) is  $-73.6(1.1)$ . If the standard assump-

tion that the top quark mass is 45 GeV and the Higgs mass 100 GeV is made, the radiatively corrected value of the weak charge  $Q_W$  is then<sup>3</sup>

$$Q_W = -71.8(1.1). \quad (15)$$

Since the experiments actually measure a ratio of the PNC amplitude to the vector part of the Stark polarizability,  $\beta$ , we need a value for  $\beta$ , which we take to be<sup>18</sup>

$$\beta = 27.2(4)a_0^3. \quad (16)$$

Combining these terms leads to the prediction for the ratio of the  $6s \rightarrow 7s$  PNC amplitude to  $\beta$ ,

$$A = 1.65(3)_{\text{expt}}(8)_{\text{theor}} \text{ mV/cm}, \quad (17)$$

which is to be compared with the presently available measurements

$$A_{\text{expt}} = 1.65(13) \text{ mV/cm (Ref. 6)}, \quad (18)$$

$$A_{\text{expt}} = 1.56(17)(12) \text{ mV/cm (Ref. 5)}. \quad (19)$$

The first error in Eq. (17) refers to the uncertain value of the Weinberg angle, and the second is our estimate of atomic structure uncertainty, to be discussed below. One can infer from the first measurement a value for the Weinberg angle, which is

$$\sin^2\theta_W = 0.229(24)_{\text{expt}}(16)_{\text{theor}}. \quad (20)$$

Significant improvement in the experimental result is expected soon,<sup>19</sup> so the question of the accuracy of the theoretical prediction is raised, and we now turn to a discussion of this issue.

The only statement about error that we can make with certainty is that the calculation presented here is precisely analogous to calculations of parity-conserving atomic properties<sup>15</sup> that are accurate to 2.9% for the  $6s$  hyperfine splitting, to 4.8% for the  $7s$  hyperfine splitting, and to 2.8% for the  $6s \rightarrow 6p$  transition amplitudes. It is in this sense that we assign an error of 5% to the theoretical value presented here. It is worth noting that the three standard calculations above involved larger shifts than the PNC calculation: for example, the change from lowest-order  $6s$  hfs to the RPA level is +12.5%, while the additional change due to Brueckner orbitals was +28%. By contrast, the lowest-order PNC result changes by only -4% on adding RPA corrections, and by +6.4% upon addition of the Brueckner-orbital corrections. For this reason the present result may be more accurate than 5%. On the other hand, as one can see from Table I, the relatively small size of the third-order corrections results from a cancellation between various similar terms, giving a final result that is an order of magnitude smaller than the individual contributions. If this detailed cancellation does not occur in higher order then our error estimate may be too optimistic. There is at least one approach towards making a more quantitative statement about the accuracy of the calculation, and that is to perform a complete third-order calculation of the standard properties listed above. There are, in addition to the numerically dominant third-order corrections included above, a large number of smaller terms. These

terms are somewhat analogous to the internal substitutions discussed above inasmuch as the one-body operator acts inside a Brueckner-orbital correction. The evaluation of these terms, which enter at the few-percent level, is presently in progress. If matrix element calculations improve to the 1% level upon the inclusion of such terms, and if the analogous PNC terms enter at under the 1% level, we would take this as evidence that our result is valid at roughly this level.

We now turn to a discussion of a major discrepancy between our prediction and another calculation that includes the Brueckner-orbital effects considered here, that of Dzuba *et al.*<sup>12</sup> Their result of  $0.90iea_0 \times 10^{-11}Q_W / -N$  is smaller than ours by 5.7%, which is significantly greater than their estimated theoretical error (2%) and much greater than our numerical error (0.2%). There are two possible sources of the disagreement, one numerical and one involving the implementation of MBPT. While the present calculation is restricted rigorously to the subset of third-order terms associated with Brueckner orbitals, Dzuba *et al.* include all third-order terms and in addition a subset of fifth-order terms arising from the "chaining" of Brueckner orbitals and a subset of fourth-order terms corresponding to mixtures of Brueckner-orbital and RPA effects. The authors' estimates of the sizes of these additional corrections, however, are much less than the 5.7% discrepancy between our result and theirs: they find that the chaining of Brueckner orbitals decreases their result by 2%, while the inclusion of the remaining third-order terms and the RPA-Brueckner cross terms causes a change of less than 1% in each case. Thus it appears that there is a substantial disagreement arising from purely numerical considerations.

We have previously noted<sup>15</sup> a discrepancy with the results of an earlier work by Dzuba *et al.*<sup>20</sup> concerning the evaluation of the second-order energy. In that case, formally identical calculations gave the results  $-0.14511$  a.u. (Ref. 15) and  $-0.14325$  a.u.<sup>20</sup> Subsequently we learned<sup>21</sup> that the cause of the discrepancy was the limited basis set used in Ref. 20. It is possible that this problem could propagate into the more complex calculation of the PNC matrix element in such a way as to produce discrepancy.

In summary, we present here a new calculation of the parity-nonconserving transition  $6s \rightarrow 7s$  in cesium including the effects of correlation. We find the result  $0.951iea_0 \times 10^{-11}Q_W / -N$ , with an error estimate of 5% extracted from the behavior of analogous calculations of known matrix elements of the atom. The discrepancy with the previous calculation that included correlation corrections is certainly partly due to numerical problems with the basis sets used in that calculation, and possibly also partly due to the different implementation of MBPT. Calculations needed to reduce the theoretical error have been discussed. We would like to close by remarking that, although a very specific demand is being put on our understanding of the relativistic many-body problem by the increasingly accurate measurements of PNC in cesium, this field of physics is of very great interest by itself. The spur provided to our theoretical understanding of

these systems and the calculational techniques needed to attack such problems numerically is certain to be valuable in many other branches of atomic and many-body physics.

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- <sup>1</sup>S. Weinberg, *Phys. Rev. Lett.* **19**, 1264 (1967); A. Salam, in *Elementary Particle Theory*, edited by N. Svartholm (Almqvist and Forlag, Stockholm, 1968).
- <sup>2</sup>U. Amaldi *et al.*, *Phys. Rev. D* **36**, 1385 (1987).
- <sup>3</sup>W. J. Marciano and A. Sirlin, *Phys. Rev. D* **27**, 552 (1983).
- <sup>4</sup>R. R. Lewis and W. Williams, *Phys. Lett.* **59B**, 70 (1975); E. Hinds and V. Hughes, *ibid.* **67B**, 487 (1977).
- <sup>5</sup>M. A. Bouchiat *et al.*, *Phys. Lett.* **117B**, 358 (1982); **134B**, 463 (1984).
- <sup>6</sup>S. L. Gilbert, M. C. Noecker, P. N. Watts, and C. E. Wieman, *Phys. Rev. Lett.* **55**, 2680 (1985); *Phys. Rev. A* **34**, 792 (1986).
- <sup>7</sup>P. Drell and E. D. Commins, *Phys. Rev. A* **32**, 2196 (1985); C. E. Tanner and E. D. Commins, *Phys. Lett.* **56**, 332 (1986).
- <sup>8</sup>T. P. Emmons, J. M. Reeves, and E. N. Fortson, *Phys. Rev. Lett.* **51**, 2089 (1983).
- <sup>9</sup>J. H. Hollister *et al.*, *Phys. Rev. Lett.* **46**, 643 (1981).
- <sup>10</sup>A.-M. Mårtensson-Pendrill, *Phys. Scr.* **36**, 122 (1987).
- <sup>11</sup>C. Bouchiat and C. A. Piketty, *Europhys. Lett.* **2**, 511 (1986).
- <sup>12</sup>V. A. Dzuba, V. V. Flambaum, P. G. Silvestrov, and O. P. Sushkov, *J. Phys. B* **18**, 597 (1985); **20**, 3297 (1987).
- <sup>13</sup>A.-M. Mårtensson-Pendrill, *J. Phys. (Paris)* **46**, 1949 (1985).
- <sup>14</sup>W. R. Johnson, D. S. Guo, M. Idrees, and J. Sapirstein, *Phys. Rev. A* **34**, 1043 (1986).
- <sup>15</sup>W. R. Johnson, M. Idrees, and J. Sapirstein, *Phys. Rev. A* **35**, 3218 (1987); Carl Wieman (private communication).
- <sup>16</sup>W. R. Johnson, S. A. Blundell, and J. Sapirstein, *Phys. Rev. A* (to be published).
- <sup>17</sup>I. Lindgren and J. Morrison, in *Atomic Many-Body Theory*, Vol. 13 of *Springer Series in Chemical Physics*, edited by V. I. Goldanskii, R. Gomer, F. P. Schäfer, and J. P. Toennies (Springer, Berlin, 1982). A relativistic generalization is given by E. Lindroth, J.-L. Heully, I. Lindgren, and A.-M. Mårtensson-Pendrill, *J. Phys. B* **20**, 1679 (1987).
- <sup>18</sup>W. R. Johnson and Z. W. Liu, *Phys. Lett. A* **119**, 407 (1987). This paper calculates the scalar Stark polarizability  $\alpha$ : the vector polarizability  $\beta$  is a factor of  $-9.9(1)$  smaller.
- <sup>19</sup>Carl Wieman (private communication).
- <sup>20</sup>V. A. Dzuba, V. V. Flambaum, and O. P. Sushkov, *J. Phys. B* **16**, 715 (1983).
- <sup>21</sup>V. A. Dzuba, V. V. Flambaum, and O. P. Sushkov (private communication).