Parity Nonconservation in the $6s^2\,{}^1S_0 \rightarrow 6s5d\,{}^3D_1$ Transition in Atomic Ytterbium

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The $6s^2\,{}^1S_0 \rightarrow 6s5d\,{}^3D_1$ transition in atomic Yb is proposed for use in the study of atomic parity nonconservation (PNC). This transition is shown to have a very large $E1$ amplitude arising from PNC: $|\mathrm{Im}(E1_{\mathrm{PNC}})| \cong 1.1 \times 10^{-9} e a_0$, and also a strongly suppressed $M1$ amplitude and a moderate Stark-induced amplitude. Extremely high-precision measurements of PNC in Yb appear possible, using experimental techniques of proven utility. Comparison of PNC in the wide range of stable isotopes of Yb may provide a unique test of the standard model of electroweak interactions.

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Precise measurements of atomic parity nonconservation (PNC) provide stringent tests of the standard model of electroweak interactions, with uncertainties usually dominated by imprecise knowledge of atomic structure. As was noted in [1], measurements of atomic PNC in a chain of isotopes of the same atom would be useful, since atomic structure uncertainties cancel in the ratio of the PNC effect in different isotopes. Such measurements would differ from those for a single isotope in several ways. First, it becomes necessary to measure PNC in individual isotopes in the chain to extremely high precision, since the fractional change in PNC effects between two isotopes with neutron numbers N and $N + \Delta N$ is small, i.e., $\approx \Delta N/N$; this also makes elements with the widest possible range of accessible isotopes attractive. Second, isotopic PNC ratios are more sensitive to different radiative corrections than those that affect single-isotope measurements, yet they retain the sensitivity of single-isotope atomic PNC to new tree-level interactions (e.g., new Z bosons) [2,3]. Thus, in combination with precise high-energy electroweak measurements, isotopic ratio measurements provide an unambiguous test for the existence of such new tree-level interactions. (This is in contrast to single-isotope PNC measurements, which can also be affected by radiative correction terms relatively inaccessible to high-energy measurements.) Finally, the interpretation of isotopic ratio measurements in terms of the standard model would at present be limited by imperfect knowledge of nuclear neutron distributions [3]. For instance, it has been shown in the cases of Pb (with $\Delta N/N = 6/126$) [3] and CS (for unstable isotopes with $\Delta N/N = 14/78$) [4] that this would be the source of an uncertainty of $\sim 1\%$ in the determination of $\sin^2\theta_W$ (where θ_W is the weak mixing angle). This is comparable to the limits from the best single-isotope measurements, due to atomic structure uncertainties. More accurate measurements of isotopic PNC ratios would be interpreted as a measurement of neutron distributions, which are otherwise difficult to determine experimentally.

It is shown here that a favorable situation occurs in the $6s^2\,{}^1S_0 \rightarrow 6s5d\,{}^3D_1$ transition (408 nm) in atomic Yb ($Z = 70$) (see Fig. 1). (Similar transitions in Ba [5] and Sm [6,7] have also been discussed as potential candidates for the study of PNC.) In Yb, the PNC-induced $E1$ amplitude is very large, while the $M1$ amplitude is strongly suppressed and the Stark-induced $E1$ amplitude is of moderate size. Hence the transition may be studied conveniently by the well-developed technique of Stark-PNC interference. Also, Yb has a wide range of stable isotopes, including both even-even $I = 0$ and odd-neutron-number, nonzero-nuclear-spin types (^{176}Yb, 12.73% natural abundance; ^{174}Yb, 31.84%; ^{173}Yb, $I = \frac{5}{2}$, 16.08%; ^{172}Yb, 21.82%; ^{171}Yb, $I = \frac{1}{2}$, 14.27%; ^{170}Yb, 3.03%; and ^{168}Yb, 0.135%). It will be shown that an experimental accuracy of $\sim 10^{-4}$ in the measurement of PNC in single isotopes of Yb with $A = 170-176$ is feasible. Measurements of PNC at this level of accuracy would, in the absence of nuclear structure uncertainties,

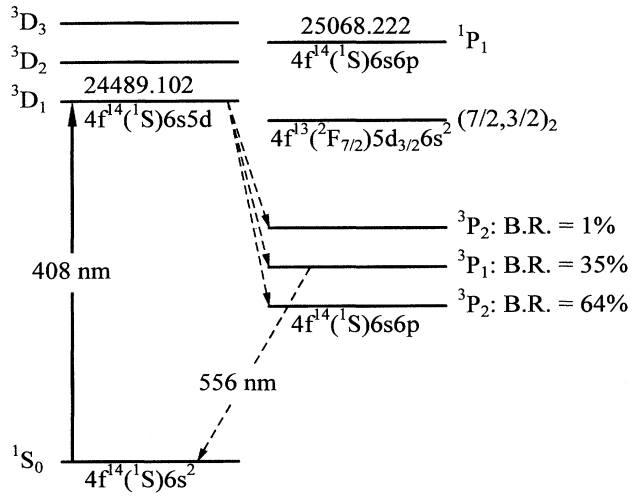

FIG. 1. Low-lying energy levels of Yb (not to scale), and radiative decay channels of the $6s5d\,{}^3D_1$ state.

lead to a determination of $\sin^2\theta_W$ with fractional uncertainty $\lesssim 0.5\%$. It is expected [8] that uncertainties in neutron distributions will limit the interpretation at the level of $\lesssim 1\%$; however, explicit nuclear structure calculations are clearly necessary, and these are underway [8]. Finally, measurements of PNC differences between different hyperfine components of the transition in the odd isotopes should allow measurement of the PNC nuclear anapole moment [9]. In what follows, however, only nuclear-spin-independent PNC effects are discussed.

The PNC-induced $E1$ amplitude is given by

$$E1_{\mathrm{PNC}} \equiv \langle 6s5d\,{}^3D_1|z|6s^2\,{}^1S_0\rangle = \sum_n \left\{ \frac{6s5d\,{}^3D_1|H_{\mathrm{weak}}|n\rangle\langle n|z|6s^2\,{}^1S_0\rangle}{E({}^3D_1) - E(n)} + \frac{\langle 6s^2\,{}^1S_0|H_{\mathrm{weak}}|n\rangle\langle n|z|6s5d\,{}^3D_1\rangle}{E({}^1S_0) - E(n)} \right\}, \quad (1)$$

where n is any odd-parity state, E is an energy, and H_{weak} is the PNC weak-interaction Hamiltonian. In the nonrelativistic limit, the single-electron form of the operator H_{weak} is given by [10]

$$H_{\mathrm{weak}} = \frac{G_F}{\sqrt{2}} \frac{1}{2m_e c} \frac{Q_W}{2} \vec{\sigma} \cdot [\vec{p}\,\delta^3(\vec{r}) + \delta^3(\vec{r})\vec{p}], \quad (2)$$

where G_F is the Fermi constant, and the nuclear weak charge Q_W is given by $Q_W \equiv -N + (1 - 4\sin^2\theta_W)Z$.

The sum in Eq. (1) is dominated by a single term corresponding to PNC mixing between the $6s5d\,{}^3D_1$ state (24 489.102 cm^{-1} above the $6s^2\,{}^1S_0$ ground state) and the nearby $J = 1$ odd-parity state at 25 068.222 cm^{-1}, which has nominal configuration and term $6s6p\,{}^1P_1$ [11]. Since H_{weak} has nonzero matrix elements only between s and p electrons, there is no mixing between the dominant configurations of these levels. However, the 25 068.222 cm^{-1} odd-parity state has a large admixture of the configuration $5d6p$ [12,13]. The weak-interaction matrix element between the two-electron terms is reduced to a single-electron matrix element by requiring that the $5d$ electron remain unaffected. Noting also that H_{weak} is a pseudoscalar, and thus that only $s_{1/2}$ and $p_{1/2}$ wave functions mix, it is convenient to express the states in the j-j coupled basis. Here, the $6s5d\,{}^3D_1$ state is written as $6s_{1/2}5d_{3/2}$, which couples through H_{weak} to the $6p_{1/2}5d_{3/2}$ terms of the odd-parity state. The dominant term in Eq. (1) then takes the form

$$E1_{\mathrm{PNC}} = b \frac{\langle 6s_{1/2}|H_{\mathrm{weak}}|6p_{1/2}\rangle\langle 6s6p\,{}^1P_1|z|6s^2\,{}^1S_0\rangle}{589\ \mathrm{cm}^{-1}}, \quad (3)$$

where the coefficient b includes both the configuration mixing amplitude and the relevant angular mixing coefficients. In [12], b is calculated to have the value 0.29. However, that calculation did not include configuration mixing of core-excited states into the odd-parity state, which is known to contribute ~20% [13,14]. Thus, in this calculation, $b = 0.26$ is assumed. The uncertainty in b is not obtainable from available experimental information. However, it may be noted that similar values for b were found with two very different calculational techniques [12,13]. In addition, similar calculations for configuration mixing in Ba give excellent agreement with experimental values for oscillator strengths that are particularly sensitive to $6s6p$-$5d6p$ mixing (see, e.g., [15]). Hence, it seems conservative to assign to b an uncertainty of ~25%, and $b = 0.26(7)$ is used in this calculation.

The value of the single-electron matrix element of H_{weak} depends on the values of the s- and p-electron wave functions and their derivatives at the nucleus. It has been shown that these values can be parametrized in terms of effective radial quantum numbers ν [10], even in complex multielectron atoms such as Pb and Bi [16,17]. The matrix element is expressed as [10]

$$\langle ns_{1/2}|H_{\mathrm{weak}}|np_{1/2}\rangle = i\frac{G_F m_e^2 \alpha^2}{\pi\sqrt{2}} \frac{Z^2 R}{(\nu_s\nu_p)^{3/2}} \frac{Q_W}{2} \mathcal{R}, \quad (4)$$

where α is the fine-structure constant and $\mathcal{R}$ is the Rydberg constant. R, the "relativistic enhancement factor," is given by

$$R = 4\frac{(a_0/2Zr_0)^{2-2\gamma}}{\Gamma^2(2\gamma+1)}, \quad (5)$$

where a_0 is the Bohr radius, $r_0 = A^{1/3} \times 1.2 \times 10^{-13}$ cm is the (approximate) nuclear radius, and $\gamma = \sqrt{1 - Z^2\alpha^2}$. For Yb, Eq. (5) yields $R = 4.0$.

The effective radial quantum numbers ν can be obtained from the binding energies of the relevant states, by using the phenomenological formula $E_b = \mathcal{R}/\nu^2$, or, alternatively, by using the hyperfine structure constants for each electron, in conjunction with phenomenological formulas for the valence electron wave functions near the nucleus [17,18]. Table I summarizes the results of various methods used to determine ν_{6s} and ν_{6p}. For the calculation of $E1_{\mathrm{PNC}}$, the following intermediate values are used: $\nu_{6s} = 1.42(8)$ and $\nu_{6p} = 1.90(18)$. The uncertainties are determined from the spread of values in Table I.

The radial matrix element in Eq. (3) is determined from the experimentally known lifetime $\tau = 5.5(5)$ ns of

TABLE I. Values of the effective nonrelativistic radial quantum numbers ν for the $6s$ and $6p$ electrons in Yb, obtained from various atomic and ionic structure parameters.

Method	ν_{6s}	ν_{6p}
$E(\mathrm{Yb}\ 6s^2\,{}^1S_0) - E(\mathrm{Yb}^+\ 6s_{1/2})$	1.48	
$E(\mathrm{Yb}\ 6s5d\,{}^3D_1) - E(\mathrm{Yb}^+\ 5d_{3/2})$	1.50	
$E(\mathrm{Yb}\ 6s6p\,{}^1P_1) - E(\mathrm{Yb}^+\ 6p_{1/2})$	1.42	
$E(\mathrm{Yb}\ 6s6p\,{}^3P_0) - E(\mathrm{Yb}^+\ 6p_{1/2})$	1.35	
hfs (Yb $6s6p\,{}^3P$)	1.41	1.73
$E(\mathrm{Yb}\ 6s6p\,{}^3P_0) - E(\mathrm{Yb}^+\ 6s_{1/2})$		1.82
$E(\mathrm{Yb}\ 6s6p\,{}^1P_1) - E(\mathrm{Yb}^+\ 6s_{1/2})$		2.08

the $6s6p\ ^1P_1$ state [19], yielding $|\langle 6a6p\ ^1P_1|z|6s^2\ ^1S_0\rangle| = 2.4(1)a_0$. Insertion of all relevant factors into Eq. (3) yields

$$|\mathrm{Im}(E1_{\mathrm{PNC}})| \cong 1.1(4) \times 10^{-9} e a_0 ; \quad (6)$$

the sign is undetermined because the sign convention of the configuration mixing coefficient b is not discussed in [12].

Contributions to the sum of Eq. (1) from terms other than the main term have also been considered. It is estimated that these change the result of Eq. (6) by $\lesssim 10\%$. For example, by far the largest additional term arises from mixing of the $6s6p\ ^3P_0$ state with the $6s^2\ ^1S_0$ ground state; this term has magnitude $\cong 8\%$ of the main term in Eq. (6). Since the relative signs cannot be determined from the available information, these additional terms are treated as an additional uncertainty, which is negligibly small compared to the other uncertainties entering the result of Eq. (6).

Stark-induced amplitudes arise because an external electric field mixes states of odd-parity into the even-parity states of interest, leading to $E1$ transitions between the perturbed states. In general, these amplitudes include scalar, vector, and tensor terms [20]. However, because the transition of interest is $J = 0 \rightarrow J = 1$, only the vector amplitude β (which arises when $\varepsilon \perp E$) is nonzero. Note also that, since the initial and final states have different total spin, this amplitude must include one nominally forbidden (singlet-triplet) radial matrix element. As in the case of $E1_{\mathrm{PNC}}$, $E1_{\mathrm{Stark}}$ is dominated by a single term arising from mixing of the $6s5d\ ^3D_1$ state with the $6s6p\ ^1P_1$ state,

$$E1_{\mathrm{Stark}} \equiv \beta E \cong e^2 E \frac{\langle 5d6s\ ^3D_1(m_J = \pm 1)|y|6s6p\ ^1P_1(m_J = 0)\rangle \langle 6s6p\ ^1P_1(m_J = 0)|z|6s^2\ ^1S_0\rangle}{E(5d6s\ ^3D_1) - E(6s6p\ ^1P_1)} . \quad (7)$$

The $^3D_1$-$^1P_1$ matrix element is dominated by the admixture of $6s6p\ ^3P_1$ into the odd-parity state, which is found to be ~ 0.14 in amplitude from the lifetime [19,21] and g value [11] of the $6s6p\ ^3P_1$ state, while the $6s5d\ ^3D_1$–$6s6p\ ^3P_1$ matrix element can be determined from the lifetime of the $6s5d\ ^3D_1$ state, which was recently measured in this laboratory [22]. These estimates yield a value for β comparable to the analogous amplitude in Cs [23] or Tl [24],

$$\beta \cong 5(2) \times 10^{-8} e a_0/(\mathrm{V/cm}), \quad (8)$$

where the uncertainty is dominated by that of the singlet-triplet mixing amplitude.

Nonzero contributions to $M1$ amplitudes in forbidden transitions in Cs and Tl—which arise due to relativistic effects, hyperfine mixing, and configuration mixing (first discussed in [10])—have been investigated in detail; see [17] for a review. For the presently discussed transition in Yb, contributions to $M1$ from relativistic effects and off-diagonal hyperfine mixing (the latter present only the odd-N isotopes) are greatly suppressed relative to the more familiar cases in Cs and Tl due the $s \rightarrow d$ nature of the transition, and are certainly $< 10^{-5}\mu_B$. Other contributions arise because the states of interest are not pure in the basis of single-configuration, L-S coupled states. $M1$ transitions occur in such a basis only between states with the same configuration and the same L and S. Thus, for a nonzero $M1$ amplitude to arise, both configuration interaction (CI, which mixes different configurations with the same L, S, and J) and spin-orbit interaction (SOI, which mixes different L and S terms of the same configuration) are necessary in *both* states of the transition. The configurations which are likely to give the largest contributions to the $M1$ amplitude are $4f^{13}5d6s6p$, $4f^{14}6p7p$, and $4f^{14}5d6d$ (configurations of the form nl^2 cannot contribute, since these have no $^3D_1$ term and so cannot mix into the $6s5d$ state in first order). Although none of the relevant CI mixings have been explicitly calculated, an order-of-magnitude argument can be given: The admixture of any of these configurations (in the "right" LS term) into the relevant states should have amplitude $\lesssim 0.1$ [11,13], and admixtures via SOI of "wrong" LS terms have typical amplitudes ~ 0.1 in Yb. This gives a crude limit of $M1 \lesssim 10^{-4}\mu_B$ due to this mechanism. Given this degree of suppression, the precise value of this amplitude is of minor importance; in the experiment suggested below, $M1$ appears only (in combination with various experimental imperfections) as a contribution to systematic effects.

The combination of a highly suppressed $M1$ amplitude and a moderate Stark-induced amplitude makes it possible to use the technique of PNC-Stark interference [25–27] to measure the PNC amplitude of the $6s^2\ ^1S_0 \rightarrow 6s5d\ ^3D_1$ transition. In fact, the experimental configuration can be closely analogous to that used in the very successful Cs PNC experiments at Boulder [27], i.e., employing an intense atomic beam of Yb, excited at 408 nm with light intensified in a standing-wave power buildup cavity, in the presence of crossed dc electric and magnetic fields. The experimental problems of most immediate concern that are not identical to those in Cs have been solved in other laboratories, e.g., the production of substantial Yb vapor pressure, of high-power cw laser light at the correct wavelength [28], and of high-quality mirrors for a power buildup cavity [29]. Since, as discussed above, the $M1$ amplitude may be somewhat

larger in Yb than in Cs, it may be necessary to further suppress systematic effects associated with this amplitude; this can be accomplished [30] by use of the geometry employed in the Tl PNC-Stark interference experiment [26] rather than the Boulder geometry. The transition can be detected by the observation of 556 nm fluorescence arising from the decay $6s5d\,^3D_1 \rightarrow 6s6p\,^3P_1 \rightarrow 6s^2\,^1S_0$ (see Fig. 1) in the excitation region, or, with higher efficiency, by probing downstream from the interaction region the metastable $6s6p\,^3P_0$ atoms which are produced in $\frac{2}{3}$ of the excitations.

The close analogy of the proposed experimental technique to previous measurements in Cs makes it possible to estimate the attainable precision reliably. Since the PNC $E1$ amplitude is ~ 100 times larger than the analogous amplitude for the $6s_{1/2} \rightarrow 7s_{1/2}$ transition in Cs [27], by analogy with the best anticipated results in Cs (i.e., at the level of $\sim 3 \times 10^{-3}$) [31] it appears possible to achieve an experimental accuracy of $\lesssim 10^{-4}$ in the measurement of PNC in single isotopes of Yb with $A = 170-176$. Preliminary to such measurements, it will be necessary to measure the Stark-induced and $M1$ amplitudes, in order to understand systematic effects in the PNC measurement; this program is now underway in this laboratory. Also, more sophisticated calculations of all relevant atomic amplitudes will be useful, and these are underway elsewhere [32,33].

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