Parity violation in atomic ytterbium

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The P-odd impurity amplitude $E1_{PNC}=-(1.15\pm0.25)\times10^{-9}i|e|a_0(-Q_w/N)$ (a_0 is the first Bohr radius, Q_w is the weak nuclear charge, and N is the number of neutrons) is calculated for the forbidden $M1$ transition $^3D_1\rightarrow{}^1S_0$ in ytterbium. The result confirms that parity-nonconservation effects are stronger in ytterbium than in cesium or thallium. The Stark amplitude $\beta=-(138\pm30)a_0^3$, required for interpreting experiments searching for P violation, is also calculated. © *1995 American Institute of Physics.*

Research on the violation of spatial parity P by atomic-physics methods has turned out to be extremely fruitful. There have been numerous experimental and theoretical studies searching for parity violation, primarily in heavy atoms.[1] So far, the most impressive results have been achieved in theoretical[2,3] and experimental[4] studies of cesium.

In the approximation of an infinitely heavy nucleon, the part of the P-odd Hamiltonian which does not depend on the nuclear spin can be written

$$H_w=-\frac{G_F}{2\sqrt{2}}Q_w\rho_p(r)\gamma_5, \tag{1}$$

where $G_F=10^{-5}/m_p^2$ is the Fermi constant, $\rho_p(r)$ is the distribution of nucleons in the nucleus, and Q_w is the weak charge of the nucleus, which is given in the standard model by

$$Q_w=-N+Z(1-4\sin^2\theta_W). \tag{2}$$

Here N and Z are the numbers of neutrons and protons in the nucleus, and θ_W is the Weinberg angle.

For the weak charge of the cesium nucleus, we now have the following value:[2–4]

$$Q_w(\mathrm{Cs}_{55}^{133})=-71.04\pm1.58\pm0.88. \tag{3}$$

The first of the errors here is experimental (primarily statistical), and the second theoretical. Taking these errors into account, we see that the magnitude of the weak charge is the same as the value of Q_w(Cs) predicted by the standard model on the basis of highly accurate measurements of the mass of the Z boson (Ref. 5): $m_Z=91.174\pm0.021$. Further progress in terms of improving the experimental and theoretical accuracy of the determination of Q_w for cesium and also in terms of seeking other atoms in which parity-violation effects are stronger than in cesium may not only lead to a more accurate test of the standard model, but also make it possible to go beyond this model and to study "new" physics.

One such atom is ytterbium, Yb ($Z=70$), which is one of the rare-earth elements. If we consider the $M1$ transition from the $^3D_1$ state to the $^1S_0$ state (this transition is obviously forbidden in the nonrelativistic limit, since the orbital quantum number L changes by 2), and if we take the P-odd electron–nucleon interaction into account, a P-odd impurity amplitude $E1_{PNC}$ arises. This amplitude is given by

$$E1_{PNC}=\sum_n \left[\frac{\langle {}^1S_0|-\mathbf{d}\boldsymbol{\varepsilon}|n\rangle\langle n|H_w|{}^3D_1\rangle}{E_{3_{D_1}}-E_n}+\frac{\langle {}^1S_0|H_w|n\rangle\langle n|-\mathbf{d}\boldsymbol{\varepsilon}|{}^3D_1\rangle}{E_{1_{S_0}}-E_n}\right]. \tag{4}$$

Here H_w is given by expression (1), $\mathbf{d}$ is the induced dipole moment of the atom, and $\boldsymbol{\varepsilon}$ is the electric component of the electromagnetic wave. The summation is to be carried out over all the intermediate states which satisfy the selection rules in terms of the total angular momentum J and the parity.

According to a semiempirical calculation by DeMille and Budker,[6] we have Im $(E1_{PNC})=1.1(4)\cdot 10^{-9}ea_0$ (e is the charge of an electron). This result is larger by a factor of about 100 than the corresponding P-odd amplitude for the $6S$–$7S$ transition in cesium. Since it is very difficult to work with a forbidden $M1$ transition, the test sample is usually (see for example Refs. 4 and 7) immersed in a static external electric field $\mathbf{E}$, which makes this transition "partly allowed." In this case a so-called Stark amplitude (E_{st}) arises; it is given by

$$E_{st}=\sum_n \left[\frac{\langle {}^1S_0|-\mathbf{d}\boldsymbol{\varepsilon}|n\rangle\langle n|-\mathbf{d}\mathbf{E}|{}^3D_1\rangle}{E_{3_{D_1}}-E_n}+\frac{\langle {}^1S_0|-\mathbf{d}\mathbf{E}|n\rangle\langle n|-\mathbf{d}\boldsymbol{\varepsilon}|{}^3D_1\rangle}{E_{1_{S_0}}-E_n}\right]. \tag{5}$$

It is not difficult to see that Stark amplitude (5) can be written in the form $E_{st}\equiv\beta i[\mathbf{E}\times\boldsymbol{\varepsilon}\,]_m$ for the transition $(|1,m\rangle\rightarrow|0,0\rangle$, where m is the projection of the angular momentum $J=1$. It follows that only the component of the light polarization which is perpendicular to the external electric field contributes to the amplitude.

Experimentally, it is customary to measure the quantity $\mathrm{Im}(E1_{PNC})/E_{st}$. According to the discussion above, one would expect this quantity to be two orders of magnitude larger in ytterbium than in cesium. In view of this strengthening, and since the experimental apparatus is almost identical to that used to study cesium or thallium, experimentalists expect to achieve an error level of better than 1% in measurements of Im $(E1_{PNC})/E_{st}$ (Ref. 6). An error at this level is interesting for two reasons. First, measurements of P-odd effects for various hyperfine components of the levels of isotopes with an odd number of neutrons (Yb^{171}, I = 1/2; Yb^{173}, I = 5/2) make it possible to determine the nuclear anapole moment. Second, it becomes possible to go beyond the scope of the standard model and to study (as we said above) new physics.

Let us elaborate. When radiation corrections (including loop corrections) to electroweak processes are taken into account, the expression for the weak nuclear charge of some arbitrary atom B with $A=Z+N$ nucleons is modified:[8]

$$Q_w(B_Z^{N+Z})=(0.9857\pm 0.0004)\rho\{-N+Z[1-(4.012\pm 0.010)\sin^2\theta_W]\}, \tag{6}$$

where $\rho=1+0.0078T$ and $\sin^2\theta_W=0.2323+0.00365S-0.00261T$.

The quantities S and T were first measured in Ref. 9 for a parametrization of "new" loop contribution in terms of effects which conserve (S) and do not conserve (T) isospin.

Working from (6), we can calculate Q_w for various ytterbium isotopes ($A=168-176$), taking the corrections S and T into account. The result is

$$Q_w(\mathrm{Yb}_{70}^{70+N}) = -91.93 \pm 0.20 - 1.01S - 0.01T + 0.986(98-N)(1+0.008T). \qquad (7)$$

Expression (7) is written in such way that the last term vanishes for the isotope with the fewest neutrons ($N=98$). It follows from (7) that the magnitude of the weak charge depends on both S and T, but it is considerably more sensitive to S. This is an important circumstance for testing various embellishments of the standard model, in particular, technicolor theories. Since the quantity T is not much greater than S in these theories ($T/S \leq 10$; Ref. 8), we can ignore the contribution of the correction T in expression (7). For models with N_T technicolors and N_D SU(2) technidoublets, the quantity S can be estimated roughly to be[8-10] $S \sim 0.1 N_D N_T$. In the minimal technicolor model (with one doublet and four technicolors) we thus have $S \approx 0.4$. In another model, with a single generation of technifermions[9] we have $S \approx 2$. We thus easily conclude that there is a good chance of finding the weak charge of ytterbium, Q_w, within $\sim 1\%$ for testing the predictions of these models.

Determining Q_w within $\sim 1\%$ will of course require, in addition to experimental measurements, a theoretical calculation of the P-odd impurity amplitude and the Stark amplitude within the specified error. The basic difficulty in improving the accuracy of calculations of the hyperfine-structure constant, the P-odd impurity amplitude, and the Stark amplitude in the case of atoms of rare-earth elements (in particular, ytterbium) is the pronounced configurational interaction and thus the need to deal with a superposition of a large number of configurations. Another problem, partly related to the first, is that of incorporating the polarization of the core. In light of the discussion above, we see that the semiempirical calculation method, which has proved so successful for cesium and thallium,[1] is not accurate enough or reliable enough in the case at hand.

We have carried out a numerical calculation of the P-odd impurity amplitude at the Stark amplitude for the isotope Yb^{173} by the method of superposition of configurations. We used the following pieces of software: 1) the HFD (Hartree–Fock–Dirac) program for calculating relativistic one-electron wave functions;[11] 2) a program for superimposing configurations, which makes it possible to find the wave function of the given atomic state as a linear combination of Slater determinants constructed from one-electron wave functions;[12] and 3) a program for calculating a one-particle density matrix and also the matrix elements for transitions between the states under consideration. The method of superposition of configurations has been used successfully in calculations on the dysprosium atom (see Ref. 13, where the method is discussed in more detail).

The ytterbium states of interest here ($^1S_0$ and $^3D_1$) are determined by the configurations $5p^6 4f^{14} 6s^2$ and $5p^6 4f^{14} 6s5d$, respectively. Amplitudes (4) and (5) are dominated by an admixture of the $^1P_1$ level, which is separated from $^3D_1$ by an energy interval of 579 cm^{-1}. The $^1P_1$ term belongs to the $5p^6 4f^{14} 6s6p$ configuration, but there is an admixture of the $5p^6 4f^{14} 6p5d$ configuration in it,[6] because of a pronounced configurational interaction (at a level of 15–17%). As a result, the one-electron matrix elements $\langle 6p|H_w|6s\rangle$ contribute to the P-odd impurity amplitude; this circumstance determines the magnitude of the effect.

In calculating the P-odd and Stark amplitudes, we note that—although the summation in (4) and (5) is formally over all states which satisfy the selection rules, including the continuum—it turns out that we can actually restrict these sums to just a few P terms, namely, those which lie closest to the $^1S_0$ and $^3D_1$ levels. The admixture of the $^1P_1$ level dominates the amplitudes. For the other P terms, the energy denominators are larger by at least an order of magnitude.

Treating the nucleus as a uniformly charged sphere, i.e., assuming

$$\rho_p(r)=\frac{3}{4\pi R^3}\,\Theta(R-r),\quad R\approx A^{1/3}\times 1.2\times 10^{-13}\ \text{cm},$$

and using Eqs. (4) and (5), we find the following results (after some calculations which will be reported in detail elsewhere):

$$E1_{PNC}=-(1.15\pm 0.25)\times 10^{-9}i|e|a_0\left(-\frac{Q_w}{N}\right), \tag{8}$$

$$\beta=-(138\pm 30)a_0^3. \tag{9}$$

In calculating these quantities, we considered the polarization of the core (the excitation of electrons from the $5s$, $5p$, and $4f$ shells), in addition to superimposing valence configurations. The contribution of the $5p^54f^{14}6s^25d$ configuration to the $^1P_1$ term turns out to be very important, causing a change of about 40% in the P-odd amplitude. At first glance, this result is surprising, since this configuration lies very high on the energy scale. However, we note that the $^3D_1$ ground configuration of the term $(5p^64f^{14}6s5d)$ is obtained from the $5p^54f^{14}6s^25d$ configuration by the one-electron transition $6s$–$5p$. Consequently, the amplitude of this configuration (~ 0.04) contributes to the expression for $\langle ^1P_1|H_w|^3D_1\rangle$—not the square of this amplitude, which is indeed small. We should also note that the reduced matrix element $\langle 5p\|H_w\|6s\rangle$ is larger than $\langle 6p\|H_w\|6s\rangle$ by a factor of 4–5.

Setting $N=103$, $Z=70$, and $\sin^2\theta_W=0.232$, and substituting into (2) and (8), we find $E1_{PNC}\approx -1.1\times 10^{-9}i|e|a_0$. This result agrees very well with the result found by a U.S. group.[6]

It can be seen from (8) and (9) that the error of our method is about 20%. The problem is that the number of Slater determinants required for constructing a more accurate wave function is much higher than the 40 000–50 000 which we are able to take into account. Improvements in accuracy can be achieved primarily by making certain modifications in our programs and also by using computers more powerful than the 486 IBM PC on which the present calculations were carried out.

Knowing $E1_{PNC}$ and β, we can easily find their ratio

$$\mathrm{Im}\,\frac{E1_{PNC}}{\beta}\approx 40.8\ \ (\text{mV/cm}). \tag{10}$$

As was mentioned earlier, the Stark amplitude (E_{st}) is dominated by the amplitude of the $E1$ transition $^1P_1\rightarrow{}^1S_0$. For the reduced matrix element we find

$$\langle ^1S_0\|er\|^1P_1\rangle\approx -5.6\,ea_0. \tag{11}$$

Using the expression for calculating the probability for the transition $\gamma,J\to\gamma',J'$ (Ref. 14),

$$W(\gamma'J',\gamma J)=\frac{2\omega^3}{3}\frac{1}{2J+1}|\langle\gamma'J'\|er\|\gamma J\rangle|^2, \tag{12}$$

where $\omega=2\pi\nu$ is the frequency of transition between the final state and the initial state, we find $W=1.67\times10^8\ s^{-1}$ for the $E1$ transition $^1P_1\to{}^1S_0$. Since the probabilities for the decay of the $^1P_1$ state into other states is negligible in comparison with that for decay to the ground state,[15] we can find the lifetime τ of the $^1P_1$ state: $\tau=1/W=6.0$ ns. Since the experimental values of τ (Ref. 16) lie in the interval 5.1–5.8 ns, we see that the agreement is completely satisfactory.

We can thus conclude that this calculation confirms that P-odd effects in ytterbium are stronger than those in cesium or thallium, so it is legitimate to speak in terms of "new" physics. We have calculated the P-odd impurity amplitude within an error about half that of Ref. 6. We have calculated the Stark amplitude, which is necessary for interpreting experiments. We have found the value of the amplitude of the $E1$ transition from the $^1P_1$ state to the $^1S_0$ state. We believe that the primary tasks now are to formulate an experiment for searching for P-parity violation in ytterbium and to improve the accuracy of theoretical calculations.

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