Precision Determination of Electroweak Coupling from Atomic Parity Violation and Implications for Particle Physics

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We carry out high-precision calculation of parity violation in a cesium atom, reducing theoretical uncertainty by a factor of 2 compared to previous evaluations. We combine previous measurements with calculations and extract the weak charge of the ^{133}Cs nucleus, $Q_W = -73.16(29)_{\rm expt}(20)_{\rm theor}$. The result is in agreement with the standard model (SM) of elementary particles. This is the most accurate to-date test of the low-energy electroweak sector of the SM. In combination with the results of high-energy collider experiments, we confirm the energy dependence (or ''running'') of the electroweak force over an energy range spanning 4 orders of magnitude (from $\sim$10 MeV to $\sim$100 GeV). Additionally, our result places constraints on a variety of new physics scenarios beyond the SM. In particular, we increase the lower limit on the masses of extra Z bosons predicted by models of grand unification and string theories.

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Atomic parity violation places powerful constraints on new physics beyond the standard model (SM) of elementary particles [1,2]. The measurements are interpreted in terms of the nuclear weak charge Q_W, quantifying the strength of the electroweak coupling between atomic electrons and quarks of the nucleus. Here we report the most accurate to-date determination of this coupling strength by combining previous measurements [3,4] with our high-precision calculations in a cesium atom. The result, $Q_W(^{133}\mathrm{Cs}) = -73.16(29)_{\rm expt}(20)_{\rm theor}$, is in a perfect agreement with the prediction of the SM. In combination with the results of high-energy collider experiments, our work confirms the predicted energy dependence (or ''running'') of the electroweak interaction over an energy range spanning 4 orders of magnitude (from $\sim$10 MeV to $\sim$100 GeV). The attained precision is important for probing ''new physics.'' As an illustration, we constrain the mass of the so-far elusive particle—the extra Z boson (Z'). Z' are hypothesized to be carriers of the ''fifth force'' of nature, and they are abundant in models of grand unification and string theories [5]. In particular, SO(10) unification predicts a Z' boson denoted as Z'_χ. A direct search at Tevatron collider [6] yielded $M_{Z'_\chi} > 0.82\ \mathrm{TeV}/c^2$. Our precision result implies a more stringent bound, $M_{Z'_\chi} > 1.3\ \mathrm{TeV}/c^2$. If Z' is discovered at the Large Hadron Collider (LHC), where the mass scale reach is somewhat higher, our result would help in exacting Z' properties.

Historically, atomic parity violation helped in establishing the validity of the SM [7–9]. While a number of experiments have been carried out, the most accurate measurement is due to Wieman and collaborators [3]. They determined a ratio of the parity nonconserving (PNC) amplitude $E_{\rm PNC}$ to the vector transition polarizability β, $E_{\rm PNC}/\beta = 1.5935(56)\ \mathrm{mV/cm}$, on the parity-forbidden electric-dipole $6S_{1/2} \to 7S_{1/2}$ transition in atomic Cs.

The measurement, however, does not directly translate into an electroweak observable of the same accuracy, as the interpretation of the experiment requires input from atomic theory. In computations, Q_W is treated as a parameter, and by combining computed $E_{\rm PNC}$ with measurements, the value of Q_W is derived. The inferred Q_W is compared with the predicted SM value, either revealing or constraining new physics. So far the atomic-theory uncertainty has been a limiting factor in this interpretation. Here we report reducing this error, leading to an improved test of the SM.

The PNC amplitude for the $6S_{1/2} \to 7S_{1/2}$ transition in Cs may be evaluated as

$$E_{\rm PNC} = \sum_n \frac{\langle 7S_{1/2}|D_z|nP_{1/2}\rangle\langle nP_{1/2}|H_W|6S_{1/2}\rangle}{E_{6S_{1/2}} - E_{nP_{1/2}}} + \sum_n \frac{\langle 7S_{1/2}|H_W|nP_{1/2}\rangle\langle nP_{1/2}|D_z|6S_{1/2}\rangle}{E_{7S_{1/2}} - E_{nP_{1/2}}}. \quad (1)$$

Here D and H_W are electric-dipole and weak interaction operators, and E_i are atomic energy levels. In the electronic sector, the effective PNC weak interaction averaged over quarks reads $H_W = -\frac{G_F}{\sqrt{8}} Q_W \gamma_5 \rho(\mathbf{r})$, where G_F is the Fermi constant, γ_5 is the Dirac matrix, and $\rho(\mathbf{r})$ is the neutron-density distribution. ^{133}Cs nucleus has $Z = 55$ protons and $N = 78$ neutrons. The value of Q_W is given approximately by $-N$.

Interpretation of the PNC measurements requires evaluating Eq. (1). Although the underlying theory of quantum electrodynamics (QED) is well established, the atomic many-body problem is intractable. Reaching theoretical accuracy equal to or better than the experimental accuracy of 0.35% has been a challenging task (see Fig. 1). An important 1% accuracy milestone was reached by the Novosibirsk [10] and Notre Dame [11] groups in the late 1980s. More recently, several groups have contributed to

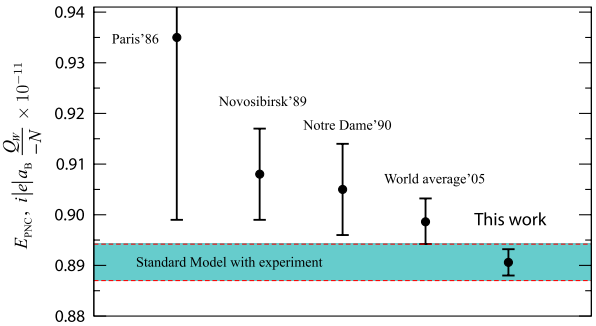

FIG. 1 (color online). Progress in evaluating the PNC amplitude. Points marked Paris '86, Novosibirsk '89, Notre Dame '90 correspond to Refs. [10,11,31]. Point marked World average '05 is due to efforts of several groups [12–16] on sub-1% Breit, QED, and neutron-skin corrections reviewed in Ref. [17]. The strip corresponds to a combination of the standard model Q_W with measurements [3,4]. The edges of the strip correspond to $\pm\sigma$ of the measurement. Here we express $E_{\rm PNC}$ in conventional units of $i|e|a_B(-Q_W/N)\times 10^{-11}$, where e is the elementary charge and a_B is the Bohr radius. These units factor out a ratio of Q_W to its approximate value, $-N$.

understanding sub-1% corrections, primarily due to the Breit (magnetic) interaction and radiative QED processes [12–16] (reviewed in [17]). The results of these calculations are summarized by the "World average '05" point of Fig. 1, which has a 0.5% error bar reflecting this progress. As of 2005, the sensitivity to new physics has been limited by the accuracy of solving the basic correlation problem. Here we report an important progress in solving it.

We wish to evaluate accurately the sum (1). To this end, we solve the Schrödinger equation $H|\Psi_v\rangle = E_v|\Psi_v\rangle$ and find atomic wave functions and energies. Even in classical mechanics, the simpler *three-body* problem cannot be solved in closed form. For a Cs atom, one solves for a correlated motion of 55 electrons. The problem is simplified by the fact that this atom has one loosely bound valence electron v outside a stiff closed-shell core. Because of that, the problem can be efficiently treated within the many-body perturbation theory [18]. In this treatment, the exact many-body state $|\Psi_v\rangle$ which stems from the approximate (Dirac-Fock) state $|\Psi_v^{(0)}\rangle$ is parametrized as $|\Psi_v\rangle = \Omega|\Psi_v^{(0)}\rangle$, where the many-body operator Ω is yet to be found. It is expanded into a hierarchy of single, double, triple, and higher-rank n-fold excitations. For example, double excitations (or simply doubles) result from a simultaneous scattering of two core electrons by their mutual Coulomb repulsion.

Notice that for the 55 electrons of Cs this treatment would be exact by including 55-fold excitations. However, manipulating such wave functions is impractical: for a basis set of 100 orbitals, one would require more than 100^{55} memory units. This number exceeds the estimated number of atoms in the Universe. Fortunately, contributions of high-rank excitations are strongly suppressed. Previous many-body calculations [11,19] in Cs stored only single and double excitations. Already at this level the attained accuracy for the atomic properties of Cs was at the level of 1% or better. To systematically improve the accuracy, here we take advantage of modern computing resources and additionally store and manipulate *triple* excitations. This is a substantial step. For example, previous calculations [11] used less than 100 Mb of storage, whereas our calculations required 100 Gb; this is a factor of 1000 increase in computational complexity.

Our specific scheme [17,20–22] of solving the atomic many-body problem is rooted in the coupled-cluster method [18]. We refer to our approximation as the CCSDVT scheme (coupled-cluster approximation including singles, doubles, and valence triples). Details will be provided elsewhere. The solution is *ab initio* relativistic, as near the Cs nucleus (where the weak interaction occurs) the electrons move with speeds approaching the speed of light. To minimize human errors, the CCSDVT code was developed independently by at least two persons. Complex derivations and coding were aided by symbolic algebra tools. An important proof of the code was made by computing properties of a lithium atom [22]. This atom has three electrons, making the CCSDVT approximation exact. We found in Ref. [22] that experimental data for Li were reproduced numerically with an accuracy reaching 0.01%.

Now we proceed to evaluating the PNC amplitude, Eq. (1), by directly summing over the intermediate $nP_{1/2}$ states [11]. This implies computing wave functions and energies of the $6S_{1/2}$, $7S_{1/2}$, and $nP_{1/2}$ states, forming matrix elements, and substituting them into Eq. (1). We employ a computationally expensive CCSDVT method only for matrix elements involving $n = 6, 7, 8, 9$ ("main" term) and compute suppressed contributions of $n \geq 10$ and core-excited states ("tail" term) with less accurate methods.

Our results for the PNC amplitude are presented in Table I. The upper panel of the table lists contributions due to the Coulomb interaction of electrons with the nucleus and other electrons. The lower panel summarizes well-established non-Coulomb contributions such as Breit, radiative (QED), and other smaller corrections. In particular, we use charge (proton) distribution for the

TABLE I. Contributions to the parity violating amplitude $E_{\rm PNC}$ for the $6S_{1/2} \to 7S_{1/2}$ transition in ^{133}Cs in units of $i|e|a_B(-Q_W/N)\times 10^{-11}$.

Coulomb interaction	
Main ($n = 6$–9)	0.8823(18)
Tail	0.0175(18)
Total correlated	0.8998(25)
Corrections	
Breit, Ref. [12]	−0.0054(5)
QED, Ref. [16]	−0.0024(3)
Neutron skin, Ref. [13]	−0.0017(5)
e-e weak interaction, Ref. [11]	0.0003
Final	0.8906(26)

Coulomb-correlated values and add the neutron-skin correction explicitly. Estimated uncertainties are listed in parentheses.

We start by assessing the accuracy of the employed CCSDVT approximation. This determines uncertainty of the "main" term contributing 98% of $E_{\rm PNC}$. Properties of low-energy states have previously been measured, and we quantify theory uncertainties by comparing these data with our *ab initio* results. For consistency we add QED, Breit, and nuclear-structure corrections to our Coulomb-correlated results. We find that the experimental energies are reproduced with an accuracy of 0.1%–0.3%. Dipole matrix elements enter the PNC amplitude directly and are derived from atomic lifetime measurements. Relevant dipoles are compared in the lower panel of Fig. 2; the CCSDVT values are within the error bars of the experiments. Finally, since the hyperfine constants A arise due to interactions of electrons with nuclear magnetic moments, matrix elements of the weak interaction $\langle nS_{1/2}|H_W|n'P_{1/2}\rangle$ may be tested by forming the geometric mean $\sqrt{A_{nS_{1/2}}A_{n'P_{1/2}}}$, Ref. [19]. Deviations of these combinations from experimental data are shown in the upper panel of Fig. 2. We find that the standard deviation (in the sense of Ref. [4]) of theoretical values from experiment is 0.2%.

Overall agreement of theoretical data with experiments indicates that the average accuracy of the CCSDVT approximation is 0.2% and we assign an error of 0.2% to the main term. Additionally, our semiempirical fitting to experimental energies modifies the main term by 0.2%, which is consistent with the above error estimate. Finally, the "tail" was computed using a blend of many-body approximations and we assign a 10% uncertainty to this contribution based on the spread of its value in different approximations. The final result (Table I) includes smaller non-Coulomb corrections and its uncertainty was estimated by adding individual uncertainties in quadrature. Previous calculations [11,19] report values larger by 0.9% than our 0.27%-accurate result. The difference is due to our inclusion of additional many-body effects, shown in Fig. 3. Direct contribution of triple excitations to matrix elements accounts for a 0.3% shift and dressing of matrix elements for another 0.3%. The remaining 0.3% comes from a consistent removal of QED and Breit corrections from experimental energies during the semiempirical fit.

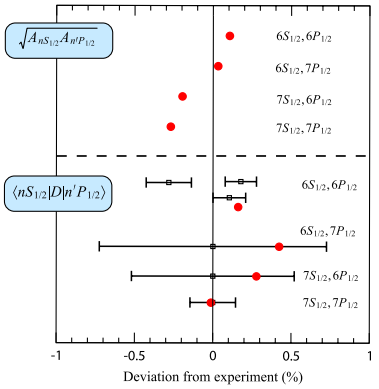

FIG. 2 (color online). Deviations of computed values (red filled circles) from experimental data (centered at zero). The upper panel displays combinations of magnetic hyperfine structure constants $\sqrt{A_{nS_{1/2}}A_{n'P_{1/2}}}$ which mimic matrix elements of the weak interaction. For these combinations, experimental error bars are negligible compared to the theoretical accuracy. The lower panel exhibits deviations of the computed dipole matrix elements from the most accurate experimental results [23,32].

With the computed $E_{\rm PNC}$ we proceed to extracting the electroweak observable. The experiment [3] determined the ratio $E_{\rm PNC}/\beta = 1.5935(56)$ mV/cm, β being the vector transition polarizability. The most accurate value of β comes from a combined determination [4,19], $\beta = -26.957(51)a_B^3$. With this β, we arrive at the nuclear weak charge

$$Q_W(^{133}\mathrm{Cs}) = -73.16(29)_{\rm expt}(20)_{\rm theor}, \qquad (2)$$

where the first uncertainty is experimental and the second uncertainty is theoretical. Taking a weighted average, $\beta = -26.99(5)a_B^3$, of two determinations [4,23] results in $Q_W(^{133}\mathrm{Cs}) = -73.25(29)_{\rm expt}(20)_{\rm theor}$. Both values are in a perfect agreement with the prediction of the SM, $Q_W^{\rm SM} = -73.16(3)$ of Ref. [24].

Our result plays a unique, and at the same time complementary, role to collider experiments. For a ^{133}Cs atom the relevant momentum transfer is just $\sim$30 MeV [15], but the exquisite accuracy of the interpretation probes minute contributions of the sea of virtual (including so-far undiscovered) particles at a much higher mass scale. The new physics brought by the virtual sea is phenomenologically described by weak isospin-conserving S and isospin-breaking T parameters [25]: $\Delta Q_W = Q_W - Q_W^{\rm SM} = -0.800S - 0.007T$. At the 1σ level, our result implies $|S| < 0.45$. Parameter S is important, for example, in indirectly constraining the mass of the Higgs particle [25]. Similarly, the extra Z boson, Z'_χ, discussed in the introduc-

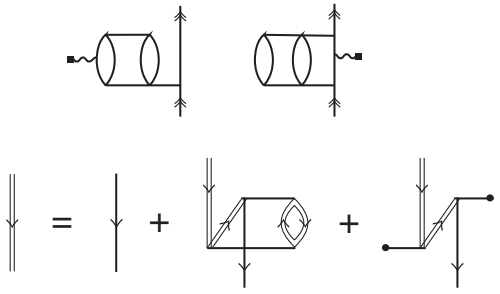

FIG. 3. Many-body diagrams responsible for the shift of the PNC amplitude compared to previous calculations. Top row: Sample direct contributions of valence triples to matrix elements (wavy capped line) [21]. Bottom row: Iterative equation for line dressing of the hole line in expressions for matrix elements [20] (similar equation holds for particle lines; exchange diagrams are not shown).

tion, would lead to a deviation [1] $\Delta Q_W \approx 84(M_W/M_{Z'_\chi})^2$, where M_W is the mass of the W boson. Our result implies a 50% chance that there is Z' (i.e., $\Delta Q_W > 0$). We find (at 84% confidence level, including $M_{Z'_\chi} = \infty$) $M_{Z'_\chi} > 1.3\ \mathrm{TeV}/c^2$, raising the present limit of $0.82\ \mathrm{TeV}/c^2$ from direct searches at Tevatron collider [6]. Our raised bound on the Z' mass carves out a lower-energy part of the discovery reach of the LHC.

Our result confirms fundamental "running" (energy dependence) of the electroweak force [26,27]. The interaction strength of particles depends on their relative collision energy E: at higher energies the collision partners tend to penetrate deeper inside the shielding clouds of virtual particles surrounding the particles. According to the SM, the interaction strength at low energies differs by about 3% from its measured value at 100 GeV. Compared to collider experiments, our result provides a reference point for the least energetic electroweak interactions. Notice that the previous analyses [16,17] of PNC in Cs were consistent with no running [28]. With our Q_W, we find the effective interaction strength (we use scheme of Ref. [29]), $\sin^2\theta_W^{\mathrm{eff}}(E \to 0) = 0.2381(11)$, θ_W being the Weinberg angle. The uncertainty is somewhat better than that of the previous most precise low-energy test of the electroweak sector obtained in the electron scattering experiment at SLAC [30]. Our result is in agreement with the SM value [29] of 0.2381(6). While an earlier evidence for running of $\sin^2\theta_W$ has been obtained at SLAC [30], the prediction of the SM was outside of their error bars. In this regard, in addition to placing important constraints on new physics beyond the SM, Cs PNC provides a higher-confidence confirmation of the predicted running of the electroweak coupling at low energies. In combination with the results of high-energy experiments at SLAC and CERN [24], this work confirms the predicted running of the electroweak interaction over an energy range spanning 4 orders of magnitude (from $\sim$10 MeV to $\sim$100 GeV).

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