Zemach Moments for Hydrogen and Deuterium

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Abstract

We determine the Zemach moments of hydrogen and deuterium for the first time using only the world data on elastic electron-proton and electron-deuteron scattering. Such moments are required for the calculation of the nuclear corrections to the hyperfine structure of these hydrogenic atoms. We compare the resulting HFS predictions to the available high-precision data and provide an estimate of the size of the nuclear polarization corrections necessary to produce agreement between experimental HFS and theoretical calculations.
**Introduction.** Nuclear and atomic size scales differ by nearly five orders of magnitude, which makes nuclear corrections to atomic energy levels very tiny. The exceptional precision of modern microwave and optical measurements of atomic level spacings nevertheless makes these nuclear effects significant. The recent measurement\[1\] of the 1S-2S interval in hydrogen to an unprecedented accuracy of 2 parts in $10^{14}$ is affected in the tenth significant figure by the finite size of the proton, and this explains the strong interest of the atomic physics community in the value of the proton’s r.m.s. charge radius\[2, 3\]. The situation for the deuterium atom is similar.

The cloudy history of experimental values for the proton radius has recently been clarified by a comprehensive analysis\[4\] of all the world’s electron-proton scattering data. That work separated the charge and magnetic scattering, incorporated (significant) Coulomb corrections\[5\], and carefully treated systematic (as well as statistical) uncertainties. The resulting value of $\langle r^2 \rangle_p^{1/2} = 0.895(18)$fm is significantly higher than most older values, and is in line with values obtained from analyses of the Lamb shift in atomic hydrogen\[6, 7, 2\]. With the inclusion of sufficiently large QED corrections of order $\alpha^8$\[7, 8\] it should soon be possible to extract values of the proton radius from the hydrogen 1S-2S interval that are an order of magnitude more precise than that of Ref.\[4\]. Even more precise values of the proton radius might result from the ongoing PSI experiment to measure the Lamb shift in muonic hydrogen\[9\].

The other area where the finite size (or internal structure) of the proton plays a significant role is the hyperfine structure of the nS levels of hydrogen. A combined analysis of various experiments measuring the 1S hyperfine splitting is given in Ref.\[10\], which advocates a value

$$\Delta E_{\text{hfs}}^\text{exp} = 1\,420\,405.751\,768(1) \, \text{kHz}$$

that has an accuracy of better than one part in $10^{12}$. The size of the proton affects the sixth significant figure. It is the magnetic nature of the hyperfine interaction that leads to this enhanced sensitivity to nuclear (i.e. short-range) properties. Hyperfine structure is much more sensitive than the Lamb shift to the high-frequency components of the electromagnetic interactions that bind atoms.

The hyperfine mechanisms are traditionally divided into three categories: pure QED, recoil, and nuclear size and structure. The pure QED contributions are listed and discussed in Refs.\[2\] and \[11\], and uncalculated terms are expected to be significantly smaller that 1 ppm relative to the Fermi hyperfine splitting. Recoil (or nuclear-mass-dependent) terms\[12\] are usually
lumped together with the nuclear corrections. Because of the sensitivity to high-frequency or short-range interaction terms, QED for systems with a fundamental anomalous magnetic moment is not renormalizable, and as a result some recoil corrections are divergent without nuclear form factors. Although nominally the same size as the static nuclear-size correction \( \text{i.e.} \) the Zemach correction\[13\] of about \(-40\) ppm relative to the Fermi hyperfine splitting and discussed below), the leading-order recoil correction is substantially smaller (about \(5\) ppm) and has only a logarithmic dependence on nuclear structure, which produces a rather smaller uncertainty, as well\[2\].

Although one would naively expect (in analogy with the Lamb shift) that for HFS the leading-order nuclear-size correction is given by a simple average over the nuclear magnetic density, this is not the case. The leading-order nuclear size and structure corrections for hyperfine splittings actually arise from two-photon-exchange diagrams and are usually divided into contributions from elastic and inelastic nuclear intermediate states (plus appropriate nuclear seagull terms). The inelastic contributions (polarization corrections) can be expressed as integrals over the spin-dependent electron-scattering structure functions\[14\], \(g_1\) and \(g_2\), and are very difficult to calculate reliably\[15, 16, 17\]. An upper limit of \(\pm 4\) ppm exists\[14\], although calculations using resonance models and existing data find smaller values (typically \(1-2\) ppm)\[17\]. The nuclear-structure-dependent corrections for the proton are therefore completely dominated by the elastic part, and that is the purview of this work.

For the \textit{deuteron} the HFS is also known with excellent accuracy\[10\]

\[\Delta E_{\text{exp}} = 327\,384.352\,522(2)\text{ kHz}\]

where nuclear effects amount to about \(138\) ppm. The deuteron presents a very different theoretical problem based on very different scales. Because the deuteron is so loosely bound it is very susceptible to breakup reactions. The deuteron Zemach correction is about \(-100\) ppm (see below), leaving an inelastic contribution of about \(240\) ppm. The bulk of the nuclear-size corrections to hyperfine structure is therefore generated by inelastic contributions\[20\], although the elastic contribution is clearly important, particularly in view of the cancellation. It is extremely valuable for any theorists attempting to perform these calculations to be able to judge the quality of their work by comparison to appropriate experimental results. For this reason we also determine the Zemach moment for the deuterium atom, even though it is not the dominant part of the nuclear contribution.
**Zemach moments.** The bulk of the electron-nucleus magnetic interaction is short ranged and confined to the vicinity of the nucleus. This is also the only region of the electron’s wave function that is significantly affected by the nuclear charge distribution, and the leading-order size effect was shown by Zemach\cite{13} to depend on the product of the proton’s elastic charge and magnetic form factors (a convolution in configuration space) in the form

$$\Delta E_{\text{Zemach}} = -2 Z \alpha m \langle r \rangle (2) E_F$$

where $E_F$ is the Fermi hyperfine splitting, $m$ is the electron mass, $Z$ is the nuclear charge, $\alpha$ is the fine-structure constant, $G_E(q^2)$ ($G_M$) is the charge (magnetic) form factor depending only on the momentum transfer (squared), $q^2 > 0$. The subtraction term $(-1)$ is necessary in order to avoid double counting the nuclear charge and magnetic moment. The convoluted configuration-space densities $\rho_{\text{ch}}$ and $\rho_{\text{mag}}$ are simple Fourier transforms of the form factors, both of which are normalized to 1 at $q^2 = 0$.

The same problems that have plagued extraction of the proton’s and deuteron’s charge radii have also complicated the calculation of $\langle r \rangle (2)$ via the momentum-space integral above. Most calculations have relied on a common dipole shape for both charge and magnetic form factors and have presented results based on various values of the single parameter in such shapes. That parameter also determines the value of the (common) mean-square radius, which historically has had well-scattered values. Results for the proton typically\cite{2} have been in the vicinity of $\langle r \rangle (2) \sim 1.0$ fm and $\Delta E_{\text{Zemach}}/E_F \sim -40$ ppm. We will use the electron-scattering data themselves, together with well-tested techniques for extracting the form factors, to evaluate $\langle r \rangle (2)$.

**Determination of $\langle r \rangle (2)$** In previous papers\cite{5, 4, 18} we have described our analysis of the world data on $e - p$ and $e - d$ scattering. Here, we use these results to determine the Zemach moments.

The proton cross sections up to the maximum momentum transfer $q_{\text{max}} = 4 fm^{-1}$ have been fit with a 5-parameter continued fraction expansion for both $G_E(q)$ and $G_M(q)$. The deuteron data up to $q_{\text{max}} = 8 fm^{-1}$ have been fit with
a 10-parameter SOG parameterization for the electric monopole (C0), magnetic dipole (M1) and electric quadrupole (C2) form factors. The references to the cross sections and polarization data included are listed in refs. [5, 4]. In the fits, the Coulomb distortion of the electron waves, neglected in all work before [5], has been included.

The separation of longitudinal (charge) and transverse (magnetization) contributions to the (e,e) cross sections is automatically performed during the fit of the cross section data. For the case of the deuteron, the separation of monopole and quadrupole contributions is also achieved as all the available polarization data are included in the data set.

An important feature of these fits is the fact that charge and magnetic form factors are simultaneously fit to the available data set. The error matrix of the fit then contains all the correlations between the two (three) form factors, resulting from the fact that the observed cross sections depend on a linear combination of charge and magnetic form factors. These correlations obviously are important when computing the uncertainty in the Zemach integral, eq. 2. As the charge/magnetic- (L/T)-separation leads to an anticorrelation between $G_E$ and $G_M$ and the Zemach moment depends on $G_E \cdot G_M$, the Zemach moment actually to some degree can be determined better than quantities depending only on $G_E$ or $G_M$, such as, e.g., the rms-radii. In order to calculate the statistical uncertainty of $\langle r \rangle_2$, we use the corresponding error matrix.

The systematic uncertainties of the data, mainly errors in the absolute normalization of the cross sections, are also affecting the uncertainty of the Zemach moments. We determine this uncertainty by changing the individual data sets by their quoted systematic uncertainty, refitting the form factors and adding quadratically the resulting changes of the Zemach moments.

From the parameterization of the data we determine the contribution to the integral eq. 2 up to $q = q_{\text{max}}$. We add the contribution from $q_{\text{max}}$ to $q = \infty$ using a dipole form factor. We have verified that, due to the smallness of the product $G_E G_M$ at large $q$, more realistic values for $G(q)$ do not make a significant difference.

The results are listed in Table I. The error bar given covers both the statistical and the systematic uncertainties of the data.

For comparison, we have also calculated the moments for some standard parameterizations of the form factors. When using for the proton the conventional dipole form factor, one finds $1.023 \text{fm}$, while the Hoehler 8.2 fit [19] gives $1.038 \text{fm}$. For the deuteron, a dipole parameterization, with the best-
Table 1: $\langle r \rangle_2$ from (e,e) data.

| Nucleus  | Zemach-moment  |
|----------|----------------|
| Proton   | 1.086±0.012 fm |
| Deuteron | 2.593±0.016 fm |

fit charge $rms$-radius determining the scale parameter, gives 2.679 fm, while the zero-range-approximation model for the deuteron of ref. [20] yields 1.708 fm.

If one calculates the deuteron charge and magnetic form factors using the impulse approximation and the AV18 potential model[21], together with a dipole nucleon form factor adjusted to give a proton Zemach moment of 1.086 fm, one finds a deuteron Zemach moment of 2.656 fm, which is about 2% too high. This illustrates an important point: the deuteron’s Zemach moment depends on a wide range of physics contributing to the charge and magnetic form factors, from the potential model used to calculate the wave functions, to possible meson-exchange currents (ignored in the impulse approximation) and relativistic corrections, and to the nucleon form factors themselves. Although the details of these ingredients are expected to produce only a small overall effect (a few percent, at most), the precision of our result for the deuteron pins down the size of the defect.

These values show that the Zemach moments are quite sensitive to the $q$-dependence of the form factors employed; they do not only depend on the $rms$-radii. The values given also show that the Zemach moments do depend appreciably on the difference between the charge and the magnetic form factors.

We note that the uncertainties on the Zemach moments are in part smaller than what could be expected from the uncertainties of the corresponding $rms$-radii [4, 18]. We attribute this to two distinct reasons: (i) the anticorrelation of $G_E$ and $G_M$ mentioned above. (ii) Sensitivity studies of the Zemach integral show that $\langle r \rangle_2$ depends on the form factors $G(q)$ up to $q \sim 3 fm^{-1}$, and not only on the low-$q$ properties (radii); at these larger $q$’s the finite-size effect in the form factors is bigger, with a correspondingly reduced importance of the systematic uncertainties of the data that dominate the uncertainty in the radii.
Hyperfine splitting. The hyperfine splitting of the 1S level of hydrogen was calculated using the fundamental constants from the 1998 CODATA evaluation\cite{22} and the QED and recoil corrections listed in Ref.\cite{2} (see also\cite{27}). We note that only the leading-order recoil correction calculated in Ref.\cite{12} is significant, because the sum of calculated recoil and structure terms of sub-leading order\cite{23} cancel almost perfectly, leaving a negligible residue\cite{2}. Our result for the Fermi splitting is 1 418 840.1 kHz, while adding in the QED and Breit corrections leads to 1 420 452.0 kHz, both results the same as that of Table XVIII of Ref.\cite{2}. Subtracting the experimental result from this theoretical result leads to a residue of 32.6 ppm of the Fermi splitting, which must accommodate all recoil and strong-interaction effects. The leading-order recoil contribution is 5.22 ppm, leaving 37.8 ppm for the sum of Zemach plus polarization corrections. Our Zemach moment correction of -41.0(5) ppm leaves the experimental result 3.2(5) ppm larger than theory without polarization. A recent calculation of the polarization correction found 1.4(6) ppm, which has the appropriate sign to complement our result, but leaves the experimental result larger than theory by 1.8(8) ppm, which is about two standard deviations from zero. This difference accounts for the smaller value of $\langle r \rangle^2$ deduced by Ref.\cite{24}, which assumed that the polarization corrections of Ref.\cite{17} are numerically accurate. Theoretical error estimates are highly subjective and the polarization corrections (or the recoil corrections) may be somewhat more uncertain than believed. Our residue of 3.2(5) ppm without polarization is within the upper limit for polarization corrections. Given the precision of our result for the Zemach moment, more attention to the polarization correction would be welcome.

The deuterium HFS involves significantly larger nuclear corrections. The QED contribution is 337 339.1 kHz, leaving a 138 ppm residue for nuclear plus recoil corrections. Our deuteron Zemach moment in Table 1 generates a -98.0(6) ppm contribution, so that polarization and recoil must contribute about 236 ppm. The reader is directed to Refs.\cite{20} and\cite{25} for a discussion of this polarization contribution which is very difficult to calculate.

Conclusion. In this paper we have determined directly from the electron scattering data the Zemach moments for the proton and the deuteron. In particular for the proton, this allows a much more precise comparison between the theoretical and experimental HFS; the present status is agreement within 1.8(8)ppm, the main source of uncertainty being the proton polarizability.
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