New Evaluation of Proton Structure Corrections to Hydrogen Hyperfine Splitting

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Abstract: We consider the proton structure corrections to hydrogen ground-state hyperfine structure, focusing on a state-of-the-art evaluation of the inelastic nucleon corrections—the polarizability corrections—using analytic fits to the most recent data. We find a value for the fractional correction \( p_{\text{pol}} \) of \( \frac{1}{3} \) ppm. This is 1–2 ppm smaller than the value of \( p_{\text{pol}} \) one would deduce using hyperfine splitting data and elastic proton structure corrections obtained from modern form factor fits. In addition, we discuss the derivations of the relevant formulas, paying attention to lepton mass effects and to questions surrounding the use of unsubtracted dispersion relations.

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1. Introduction

Hyperfine splitting (hfs) in the hydrogen ground state is measured to 13 significant figures in frequency units [1].

\[
E_{\text{hfs}}(\mathbf{p}) = 1420 \times 4057517667(9) \text{ MHz}.
\]

(1)

This accuracy is especially remarkable to theorists, who are hopeful of obtaining calculations accurate to a part per million (ppm) or so. We are close to reaching this goal, but some improvement is still needed and there currently seems to be a few ppm discrepancy between the best calculations and the data.

The main uncertainty in calculating the hfs in hydrogen comes from the hadronic, or proton structure, corrections. Calculation in this case is not \textit{ab initio} calculation, which is currently impossible, but rather calculations that relate proton structure contributions in the bound state energy to information about proton structure obtained from elastic and inelastic electron-proton scattering measurements. Historically, the elastic and inelastic contributions, the latter also called polarizability corrections have often been treated separately, with the elastic corrections further divided into a nonrelativistic Zemach term and relativistic recoil corrections. From a modern viewpoint, the elastic and inelastic corrections should be treated as a unit since the sum lacks certain ambiguities that exist in the individual terms.
This talk will focus on the polarizability contributions, but noting the last remark, discussion of the Zemach and recoil corrections will not be omitted.

2. Hyperfine splitting calculations

The calculated hyperfine splitting in hydrogen is \[ \text{E}_{\text{hf}}(e, p) = 1 + \text{QED} + \mathbf{p}_{\text{weak}} + \text{str} \mathbf{E}^p_F; \] where the Fermi energy is \[ \mathbf{E}_F = \frac{8}{3} \frac{3}{m^3} \mathbf{B}_p = \frac{8}{3m^2} \frac{m^3}{m_p} (1 + \mathbf{p}) \; ; \] with \( m = m_e m_p = m_p + m_e \) being the reduced mass (and there are hadronic and muonic vacuum polarization terms \[2\] which are included as higher order corrections to the Zemach term below). The QED terms are accurately calculated and well known. They will not be discussed, except to mention that could be obtained without calculation. The QED corrections are the same for muonium, so it is possible to obtain them to an accuracy more than adequate for the present purpose using muonium hfs data and a judicious subtraction \[4, 5\]. The weak interaction corrections \[6\] also will not be discussed, and are in any case quite small. We will discuss the proton structure dependent corrections,

\[ \text{str} = \text{el} + \text{inel} = \text{Z} + \mathbf{p}_{\text{R}} + \text{pol}; \]

where the terms on the right-hand-side are the Zemach, recoil, and polarizability corrections.

The proton structure corrections come from two-photon exchange, as diagramed in Fig. 1. Generically, the diagram consists of Compton scattering of off-shell photons from an electron knit together with similar Compton scattering from the proton. (We are neglecting the characteristic momentum of the bound electron. This allows a noticeably simpler two-photon calculation than for a scattering process \[7\]. One can show that keeping the characteristic momentum would give corrections of \( \mathcal{O}(m^2) \) smaller than terms that are kept \[8\].)

![Fig. 1. Generic two-photon exchange diagrams, giving proton-structure corrections to hyperfine splitting.](image)

If the hadronic state represented as a blob in Fig. 1 is itself just a proton, the two-photon exchange specializes to Fig. 2. The photon electron vertex is known, and we can calculate the diagram using \[9, 10\]

\[ = F_1(q^2) + \frac{1}{2m_p} \mathbf{q} F_2(q^2) \]

for the photon-proton vertex with incoming photon momentum \( q \). The functions \( F_1 \) and \( F_2 \) are the Dirac and Pauli form factors of the proton. They are measured in elastic electron-proton scattering, and we shall refer to the contribution to the hyperfine energy from Fig. 2 as the elastic contribution.

One should know that using Eq. (5) is an approximation, because this form of the vertex is sufficient and correct only when both the proton entering and leaving the vertex are on mass-shell. However, if
one is able to do the box diagram calculation using an unsubtracted dispersion relation, the on-shell parts of the elastic calculation are all that is needed. The story fits nicely into the discussion surrounding the derivation of the inelastic contributions, and we reserve its telling until we reach that discussion. For now, we will just note that the final sum of the inelastic and elastic proton structure corrections includes terms precisely as derived from the above form of the photon-proton vertex.

The elastic contributions are separated as

$$\frac{E_2}{E_F} = z + \frac{p}{r}$$

where the separation is into non-relativistic and relativistic terms—“Zemach” and “recoil.” Non-relativistic means the limit $m_p \to 1$ with $m_e$ held fixed and with proton size held fixed. (Proton size information is embedded in the form factors $F_1$ and $F_2$.)

The Zemach correction was worked out by Zemach in 1956 [11]; in modern form it is

$$z = \frac{8 m_p}{r} \int_0^1 \frac{dQ^2}{Q^2} G_E (Q^2) G_M (Q^2) \frac{1}{1 + \frac{p}{r}} = 2 m_e r_Z;$$

the last equality defining the Zemach radius $r_Z$ and we have used $Q^2 = q^2$. The charge and magnetic form factors are linear combinations of $F_1$ and $F_2$,

$$G_M = F_1 + F_2;$$
$$G_E = F_1 + \frac{Q^2}{4m_p} F_2.$$
There are two structure functions $H_1$ and $H_2$ which depend on $q^2$ and on the photon energy $\gamma$, defined in the lab frame so that $m_p = p \cdot q$.

There is an optical theorem that relates the imaginary part of the forward Compton amplitude to the cross section for inelastic scattering of off-shell photons from protons. The relations precisely are

$$\text{Im} \ H_1 (\frac{\gamma q^2}{2}) = \frac{g_1 (\frac{\gamma q^2}{2})}{(1 + p)^3 m_p}$$
$$\text{Im} \ H_2 (\frac{\gamma q^2}{2}) = \frac{m_p}{2} g_2 (\frac{\gamma q^2}{2});$$  \hspace{1cm} (11)

where $g_1$ and $g_2$ are functions appearing in the cross section and are measured [18, 19, 20, 21, 22] at SLAC, HERMES, JLab, and elsewhere.

Using the Compton amplitude in terms of $H_1$ and $H_2$, Eq. (10), in evaluating the inelastic part of the two-photon loops gives

$$\text{pol} = \frac{E_F}{E_2} \int_{\text{inel}} \frac{d^4Q}{(Q^4 + 4m_p^2Q_0^2)^2} \frac{Q Q_0^2 + Q^2}{Q_0^2} \text{Im} \ H_1 (\frac{\gamma q^2}{2})$$
$$\text{in} \ H_2 (\frac{\gamma q^2}{2})$$

where we have Wick rotated the integral so that $Q_0 = \frac{\gamma}{2}$, $Q = \frac{\gamma q^2}{2}$, and $Q^2_0 = Q^2$. Since $H_{1\beta}$ are not measured, we obtain them from a dispersion relation, which will discussed in a subsequent section.

Assuming no subtraction,

$$H_1^\text{inel} (\frac{\gamma q^2}{2}) = \frac{1}{Z} \int_{\text{th}} \text{Im} \ H_1 (\frac{\gamma q^2}{2})$$

where the integral is only over the inelastic region, and similarly for $H_2$.

Putting things together, neglecting $m_e$ inside the integral, and integrating what can be integrated, one obtains the expression

$$\text{pol} = \frac{m_e}{2(1 + p)} \left( \frac{1}{1} + \frac{2}{2} \right);$$  \hspace{1cm} (12)

where (with $Z = \frac{\gamma}{2}$),

$$1 = \frac{9}{4} \int_{\text{th}} \text{d} \frac{Q_0^2}{Q^2} F_2^2 (\frac{Q^2}{2}) + 4m_p \int_{\text{th}} \text{d} \frac{1}{2} (1) g_1 (\frac{\gamma q^2}{2});$$
$$2 = 12m_p \int_{\text{th}} \text{d} \frac{Q_0^2}{Q^2} \int_{\text{th}} \text{d} \frac{1}{2} (1) g_2 (\frac{\gamma q^2}{2});$$  \hspace{1cm} (15)

The auxiliary functions are defined by

$$1 (1) = 3 + 2 + 2 (2)^p (1) = \frac{9}{4};$$
$$2 (1) = 1 + 2 \frac{p}{(1 + 1)};$$

The integral for $1$ is touchy. Only the second terms comes from the proceedrue just outlined; it was historically thought convenient to add the first term, and then subtract the same term from the elastic contributions, specifically from the recoil corrections. This stratagem is what allows the electron mass to be taken to zero in $1$. The individual terms in $1$ diverge (they would not had the electron mass been kept), but the whole is finite because of the Gerasimov-Drell-Hearn (GDH) [23, 24] sum rule,

$$4m_p \int_{\text{th}} \text{d} \frac{1}{2} g_1 (\frac{\gamma q^2}{2}) = \frac{2}{p};$$  \hspace{1cm} (17)
coupled with the observation that the auxiliary function \( \lambda \) becomes unity as we approach the real photon point.

The polarizability expressions have some history. A short version is that considerations of \( \text{pol} \) were begun by Iddings in 1965 [12], improved by Drell and Sullivan in 1966 [13], and given in present notation by de Rafael in 1971 [14]. But no sufficient spin-dependent data existed, so it was several decades before the formula could be evaluated to a result incompatible with zero. In 2002, Faustov and Martynenko became the first to use \( g_{1,2} \) data to obtain results inconsistent with zero [16]. They got

\[
\text{pol} = (1.40 \pm 0.60) \text{ ppm}
\]

(18)

However, they only used SLAC data and \( g_1 \) and \( g_2 \) are sensitive to the behavior of the structure functions at low \( Q^2 \). Also in 2002 there appeared analytic expressions for \( g_{1,2} \) fit to data by Simula, Osipenko, Ricco, and Taiuti [25], which included JLab as well as SLAC data. They did not at that time integrate their results to obtain \( \text{pol} \). Had they done so, they would have obtained \( \text{pol} = (0.4 \pm 0.6) \text{ ppm} \) [17].

We now have enough information to discover a bit of trouble. Table 1 summarizes how things stood before the 2005/2006 re-evaluations of \( \text{pol} \). The sum of all corrections is \( 1.59 \pm 0.77 \text{ ppm} \) short of what would be desired by experimental data. Using the Simula et al. value for \( \text{pol} \) would make the deficit greater. Using other proton form factor fits (limiting ourselves to modern ones that fit the data well) in evaluating \( Z \) can reduce the deficit somewhat, but not by enough to ameliorate the problem [17].

**Table 1.** Corrections to hydrogenic hyperfine structure, as they could have been given in 2004. The first line with numbers gives the “target value” based on the experimental data and the best evaluation of the Fermi energy (8 figures) based on known physical constants. The corrections are listed next. (The Zemach term includes a 1.53% correction from higher order electronic contributions [26], as well as a +0.07 ppm correction from muonic vacuum polarization and a +0.01 ppm correction from hadronic vacuum polarization [2].) The total of all corrections is \( 1.59 \pm 0.77 \text{ ppm} \) short of the experimental value.

| Quantity | value (ppm) | uncertainty (ppm) |
|----------|-------------|-------------------|
| \( E_{\text{hfs}} \) \( p \rightarrow E_p \) \( e_p \) | 1103.49 | 0.51 |
| \( Q \) \( E \) \( D \) | 1136.19 | 0.30 |
| \( Z \) \( \text{using Friar & Sick [27]} \) | 41.59 | 0.46 |
| \( P \) \( R \) | 5.84 | 0.25 |
| \( P \) \( \text{pol} \) \( (\text{from Faustov & Martynenko [16]} \) | 1.40 | 0.60 |
| \( P \) \( \text{weak} \) | 0.06 |
| Total | 1101.90 | 0.77 |
| Deficit | 1.59 | 0.77 |

The discrepancy is not large, measured in standard deviations. On the other hand, the problem is clearly not in statistical fluctuations of the hfs measurement one is trying to explain, so one would like to do better. As listed in the Table, the largest uncertainty in the corrections comes from \( \text{pol} \). Further, the polarizability corrections require knowledge of \( g_1 \) and \( g_2 \) at relatively low \( Q^2 \), and good data pressing farther into the required kinematic regime has relatively recently become available from JLab (the Thomas Jefferson National Accelerator Laboratory, in Newport News, Virginia, USA). Accordingly, we shall present a state-of-the-art evaluation of the polarizability correction for electronic hydrogen. To give away our results [17] at the outset, we essentially confirm (remarkably, given the improvements in data) the 2002 results of Faustov and Martynenko.
3. Re-evaluation of $g_1$

Data for $g_1$ ($\gamma q^2$) has improved due to the EG1 experiment at JLab, which ran in 2005. Data based on preliminary analysis is available [22]; final data is anticipated in late 2006. A sample of the new data is shown in Fig. 3. Since a function of two variables can be complicated to show, what is shown is the integral

$$I(Q^2) = \int_{4m_p}^{2g_1(\gamma; Q^2)}$$

which differs from an integral appearing in $g_1$ in lacking the auxiliary function. The integration was done by the experimenters themselves. We remind the reader that this integral is expected to reach the Gerasimov-Drell-Hearn value $2p$ at the real photon point, and that because of cancellations the difference of this integral from $2p$ is more relevant to the final answer for $\rho_1$ than its absolute value.

Fig. 3. Data for (an integral over) the spin-dependent structure function $g_1$ ($\gamma q^2$). The data is from the EG1 experiment at Jefferson Lab from the year 2005. The Simula et al. curve is from a fit published in 2002.

All the data shown is new; there was no polarized electron-proton scattering data available below $Q^2 = 0.05$ GeV$^2$ when Simula et al. and Faustov and Martynenko did their fits. A curve obtained by integrating Simula et al.’s fit for $g_1$ is also shown on the Figure; we do not have enough information to produce a similar curve for Faustov and Martynenko’s fit.

Integration in the region $Q^2 > 0.05$ GeV$^2$ is done using analytic fits to actual data for $g_1$. For $Q^2$ below $0.05$ GeV$^2$, there is no data, so we do an interpolation based on a low $Q^2$ expansion within the integral to get (with $Q^2 > 0.05$ GeV$^2$),

$$\int_{4m_p}^{2g_1(\gamma; Q^2)} F_2 (Q^2) + 4m_p \frac{d}{dQ^2} ( )g_1 (\gamma; Q^2)$$

(20)

Here $x_P$ is from the expansion of the Pauli form factor $F_2 (Q^2) = x_P^2 + 6 + \cdots$, and the “forward spin polarizability” $\rho_0$ has been evaluated from data for other purposes [28],

$$\int_{4m_p}^{2g_1(\gamma; 0)} = [1 \Omega 1 0 \Omega 0 0 \Omega 0] 10^4 \text{ fm}^4$$

(21)

Here $\Omega$ is from the expansion of the Pauli form factor $F_2 (Q^2) = x_P^2 + 6 + \cdots$, and the “forward spin polarizability” $\rho_0$ has been evaluated from data for other purposes [28],

$$\int_{4m_p}^{2g_1(\gamma; 0)} = [1 \Omega 1 0 \Omega 0 0 \Omega 0] 10^4 \text{ fm}^4$$

(21)
The parameter $c_1$ is defined from the slope at low $Q^2$ of the integral shown in Fig. 3,

$$I(Q^2) = 4m_p \int_{\Theta_{th}} \frac{d}{d\Theta} g_1(\Theta_{th}; Q^2) = \frac{Z}{c_1} \left( \frac{Q^2}{m_p^2} \right) + 8m_p^2 c_1 Q^2 + O(Q^4);$$

we find and use $c_1 = 2.95 \pm 0.11$ GeV$^4$ [17].

We need to comment that for $g_2$, we need $g_2$, and there is almost no data for $g_2$ on the proton. One estimates $g_2$ by relating it to $g_1$ using the Wandzura-Wilczek relation [29], which we shall not detail here. Fortunately, the auxiliary function $2(\ )$ is small over the region where we need to do the integrals, so that even when we assigned 100% error bars to the contribution from $g_2$, the effect on the final answer was not great.

Our overall result is [17]

$$p_{o1} = 1.3 \pm 0.3 \text{ ppm};$$

which is similar to the Faustov-Martynenko result. This result means that the polarizability corrections no longer give the largest uncertainty in Table 1. It also means that the theory deficit outlined in Table 1 still remains, even becoming modestly larger with a smaller uncertainty limit, at $(1 \pm 0.69 \pm 0.57)$ ppm.

4. Comments on the derivations of the formulas

The polarizability corrections depend on theoretical results that are obtained using unsubtracted dispersion relations. One would like to know just what this means, and since there is at least a small discrepancy between calculation and data, one would like to be able to assess the validity of such dispersion relations.

Also, the hyperfine splitting in muonic hydrogen may be measured soon. The polarizability corrections have been calculated for this case also [30], albeit only with older fits to the structure function data and the relevant formulas, with non-zero lepton mass everywhere, are available [30] from a single source, so one would like to verify these formulas. It turns out that keeping the lepton mass does not greatly increase calculational effort or the length of the formulas, so we can do the groundwork for the muonic hfs case simultaneously with the assessment of the ordinary hydrogen hfs calculation, although we shall not here display the formulas for non-zero lepton mass.

The calculation begins by writing out the loop calculation using the known electron vertices and the definition of the Compton scattering amplitudes involving $H_1$ and $H_2$ as given in Eq. (10). One can and should use this formalism for all the hadronic intermediate states, including the single proton intermediate states. The single proton intermediate states give contributions to $H_1$ and $H_2$ that can be (more-or-less) easily calculated given a photon-proton-proton vertex such as Eq. (5). For reference, we give the result for $H_1$,

$$H_1^{el} = \frac{2m_p}{q^2 F_1(G_M (q^2) + F_2(q^2))} G_{M}(q^2) \frac{(q^2 + 1)^2}{4m_p^2} + \frac{F_2(q^2)}{4m_p^2};$$

If one is calculating only the “elastic terms,” one can use the result for $H_1^{el}$ directly in the loop calculation and obtain a result [9] that one may call $\epsilon_1$: All terms in $H_1^{el}$ will contribute, specifically including the $F_2(q^2)$ term clearly visible above. A criticism of this procedure is that the proton vertex used is not demonstrably valid when the intermediate proton is off shell, so the above expression may or may not be correct overall. However, it is correct at the proton pole.

Alternatively, one may do a unified calculation of the elastic and inelastic contributions. Since we don’t have a direct calculation of the $H_1$ for the inelastic case, we obtain them using dispersion relations. Including the elastic terms in the dispersion relation is no problem [12, 13]. One just needs the imaginary parts of $H_1^{el}$; these are easy to obtain, and contain Dirac delta-functions that ensure the elastic scattering condition $Q^2 = (2m_p)$. 

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Dispersion relations involve imagining one of the real variables to be a complex one and then using the Cauchy integral formula to find the functions $H_i$ at a particular point in terms of an integral around the boundary of some region. In the present case we “disperse” in $q^2$, treating $q^2$ as a constant while we do so. Three things are needed to make the dispersion calculation work:

The Cauchy formula and knowing the analytic structure of the desired amplitudes.

The optical theorem, to relate the forward Compton $\Im H_i$ to inelastic scattering cross sections.

Legitimately discarding contributions from some 1 contour, if the dispersion relation is to be “unsubtracted.”

The first two are not in question.

For the present case, the contour of integration is illustrated in Fig. 4, where one should imagine the outside circle having infinite radius. The result for $H_1$ begins its existence as

$$H_1(iq^2) = \frac{\text{Res}}{\text{el}} \frac{H_1(0; q^2)}{2^{\frac{d}{2}}} \left[ \frac{1}{Z} \Im \frac{H_1(0; q^2)}{2^{\frac{d}{2}}} \right] + \frac{1}{2^{\frac{d}{2}}} \int \frac{H_1(0; q^2)}{2^{\frac{d}{2}}} \left( -\frac{q^2}{2} \right) \dd \phi^2 : (25)$$

![Fig. 4. Contour in complex $q^2$ plane for applying Cauchy identity to $H_1$ or $H_2$.](image)

The numerator of the first term is the residue (Res) from the poles in $q^2$ for the elastic part of $H_1$, as from Eq. (24). Note that the $F_2$ term in $H_1(0; q^2)$, Eq. (24), is constant in $q^2$, certainly lacking a pole in $q^2$. Hence this term never enters the dispersion relation, and no $F_2$ term arises from the elastic contribution, as calculated this way.

The second term leads to the $g_1$ term in the quantity $H_1$ given earlier, after using the optical theorem to relate $\Im H_1$ to $g_1$.

The third term is the integral over the part of the contour which is the infinite radius circle. The commonly quoted results for $p_{olb}$, which appear in this talk, depend on dropping this term. The term is zero, if $H_1$ falls to zero at infinite $q^2$ Assuming this is true, however, appears to be a dramatic assumption. It fails for $H_1(0; q^2)$ alone. Hence, for the assumption to succeed requires an exact cancelation between elastic and inelastic contributions (or a failure of Eq. (24) on the big contour). On the positive side are several considerations. One is that nearly the same derivation gives the GDH sum rule, which is checked experimentally and works, within current experimental uncertainty (8%) [31]. Also, the GDH sum rule has been checked in lowest order and next-to-lowest order perturbation theory in QED, where it appears to work [32, 33]. Finally, Regge theory suggests the Compton amplitude does fall to zero with energy [34], as one would like, although Regge theory famously gave wrong high energy behavior.
for spin-independent analogs of $g_1$ and $g_2$ [35]. Hence there are indications, though not decisive proof, supporting the unsubtracted dispersion relation.

The derivation finishes by subtracting a term involving $F_2^2$ from the relativistic recoil term, so as to obtain exactly the elastic corrections $e_1 = z + \frac{p}{R}$ that were obtained (say) by Bodwin and Yennie for a calculation of the elastic terms only, using Eq. (5) at the photon-proton vertices and no dispersion theory [9]. After adding the same term to the polarizability corrections in $e_1$, one obtains the commonly quoted result for $e_1$ [13, 14, 16]. As noted earlier, this reorganization also allows $e_1$ to be finite in the $m_e! 0$ limit. Beyond the historical connection, if one is comfortable with the unsubtracted dispersion relation, the use of the dispersion theory gives a more secure result because it uses only the pole part of the photon-proton-proton vertex, so that the combined elastic and inelastic result does not depend on the general validity of whatever photon-proton-proton vertex one uses.

5. Conclusion

The evaluation of the polarizability contributions to hydrogen hyperfine structure, $\mu_{\text{pol}}$ based on latest proton structure function data is $\mu_{\text{pol}} = 1.3\pm0.3$ ppm. This is quite similar to the Faustov-Martynenko result, which we think is remarkable given the improvement in the data upon which it is based. Most of the calculated $\mu_{\text{pol}}$ comes from integration regions where the photon four-momentum squared is small, $Q^2 < 1$ GeV$^2$.

There is still a modest discrepancy between the hydrogen hfs calculation and experiment, on the order of 2 ppm. Where may the problem lie? It could be in the use of the unsubtracted dispersion relation; or it could be in the value of the Zemach radius, which taken at face value now contributes the largest single uncertainty among the hadronic corrections to hfs; or perhaps it is a low $Q^2$ surprise in $g_1$ or $g_2$. We would like to know. It is at any rate not a statistical fluctuation in the hfs data itself.

An interplay between the fields of atomic and nuclear or particle physics may be relevant to sorting out problem. For one example, the best values of the proton charge radius currently come from small corrections accurately measured in atomic Lamb shift [36]. The precision of the atomic measurement of the proton charge radius can increase markedly if the Lamb shift is measured in muonic hydrogen [37], which could happen in 2007, if the Paul Scherrer Institute accelerator schedule holds. In the present context, the charge radius is noticed by its effect on determinations of the Zemach radius.

For ourselves, a clear continuation of the present program is to finish evaluations of the muonic hydrogen ground state hfs. We have the formulas with all lepton masses in place, and are currently waiting until the final EG1 data is released, which we think will be rather soon, before publishing with a numerical evaluation.

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