Higher-Order Nuclear-Size Corrections in Atomic Hydrogen

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Abstract

Nuclear-size corrections of order \((Z\alpha)^5\) and \((Z\alpha)^6\) to the S-state levels of hydrogenic atoms are considered. These nuclear-elastic contributions are somewhat smaller than the polarizability (nuclear-inelastic) corrections for deuterium, but are of comparable or larger size for the hydrogen case. For deuterium the (attractive) nonrelativistic \((Z\alpha)^5\) correction to the 2S-1S transition is 0.49 kHz, while the (repulsive) relativistic \((Z\alpha)^6\) contribution is −3.40 kHz. For the proton the corresponding corrections are 0.03 kHz and −0.61 kHz, respectively. The \((Z\alpha)^5\) contribution largely cancels the Coulomb-retardation part of the nuclear-polarization correction.
Introduction

Recent experiments\[1, 2, 3\] have pushed the precision of the spectroscopy of the hydrogen isotopes to the point where previously unconsidered higher-order terms (in $\alpha$, the fine-structure constant) are now required. In the isotope shift of the 2S-1S transition between deuterium and normal hydrogen, for example, experimental uncertainties\[4\] of less than 0.2 kHz (one part in $3 \cdot 10^4$ of the total nuclear-finite-size correction) have been reported. The precision is such that these measurements afford us an unparalleled opportunity to extract a precise value of the d-p mean-square-radius difference. At the reported level of experimental precision, this quantity is sensitive to “exotic” contributions to the charge density\[5\], such as relativistic corrections and meson-exchange currents. It therefore behooves us to calculate all higher-order contributions to the (atomic) frequency shift of this size.

We report here a calculation of nuclear finite-size (i.e., nuclear-elastic) corrections of orders $(Z\alpha)^5$ and $(Z\alpha)^6$, which supplement the usual leading-order $(Z\alpha)^4$ term. Recently, the polarization (nuclear-inelastic) corrections of order $(Z\alpha)^5$ were calculated for deuterium\[6\] by expanding that quantity in a series in $\bar{E}R \sim \frac{1}{20}$, where $\bar{E}$ is the average (virtual) nuclear-excitation energy and $R$ is a typical nuclear size. The first three orders in this series are expected to be accurate at the level of roughly 0.01 kHz, although individual nuclear observables in that expression cannot be determined to that accuracy\[7\]. Very recently, the leading-logarithm contributions to the proton-polarizability correction were calculated\[8\], as well.

Fortunately, little analytic work is required to obtain the finite-size corrections, since they were calculated many years ago in the context of muonic atoms\[9, 10\]. The first three orders of corrections for the $n$th S-state can be written in the form:

$$\Delta E_n = \frac{2\pi}{3} Z\alpha |\phi_n(0)|^2 \left( \langle r^2 \rangle - \frac{Z\alpha\mu}{2} \langle r^3 \rangle_{(2)} + (Z\alpha)^2 F_{\text{REL}} + (Z\alpha\mu)^2 F_{\text{NR}} + \cdots \right),$$  

(1)

where $Z$ is the nuclear charge, $\langle r^m \rangle$ is the $m$th moment of the nuclear charge distribution (normalized to unit charge), $\mu$ is the reduced mass, $\phi_n(0)$ is the electron wave function at the origin, and the Zemach moment\[11, 9\] $\langle r^3 \rangle_{(2)}$ is defined by

$$\langle r^m \rangle_{(2)} = \int d^3r r^m \rho_{(2)}(r),$$  

(2)

where the convoluted (Zemach) charge density is given by

$$\rho_{(2)}(r) = \int d^3 z \rho(|z - r|) \rho(z) \equiv \rho \otimes \rho.$$  

(3)
The nonrelativistic correction $F_{NR}$ (of relative order $(Z\alpha)^2 m_e^2 R^2$, where $m_e$ is the electron mass) is negligible and will not be considered further, while the corresponding relativistic correction is defined by

$$F_{\text{REL}} = -\langle r^2 \rangle \left( \langle \ln(\beta r) \rangle + \left[ \psi(n) + \gamma - \frac{(5n + 9)(n - 1)}{4n^2} \right] + \gamma - 2 \right) + I_{\text{REL}},$$

(4)

where $\psi(n)$ is the digamma function, $\gamma$ is Euler’s constant, $\beta = 2Z\alpha\mu/n$, and

$$I_{\text{REL}} = -\frac{\langle r^3 \rangle \langle 1/r \rangle}{3}$$

$$+ \int d^3s \rho(s) \int d^3t \rho(t) \Theta(s - t) \left[ \left( t^2 + s^2 \right) \ln(t/s) - \frac{t^3}{3s} + \frac{s^3}{3t} + \frac{s^2 - t^2}{3} \right]$$

$$+ 6 \int d^3u \rho(u) \int d^3t \rho(t) \int d^3s \rho(s) \Theta(u - t) \Theta(t - s) \left[ \frac{s^2}{3} \ln(t/s) - \frac{s^4}{45tu} \right.$$

$$\left. + \frac{s^3}{9} \left( \frac{1}{t} + \frac{1}{u} \right) + \frac{s^2t^2}{36u^2} - \frac{2st^3}{9u} + \frac{s^2}{9} \right].$$

(5)

The n-dependent terms in Eq. (4) were calculated independently by Karshenboim[12].

We first treat $F_{\text{REL}}$ before discussing the smaller, nonrelativistic $(Z\alpha)^5$ contribution. We calculate $\langle r^2 \rangle$, $\langle \ln(2\alpha\mu r) \rangle$, and $I_{\text{REL}}$ using the same techniques adopted earlier to treat the nuclear-polarization observables[6]. The proton charge distribution is taken to be an exponential (dipole form factor) with a radius[13] of 0.862 fm. All integrals are known analytically for this case[9]. The deuteron charge distribution is obtained by first solving for the deuteron wave function using a variety[14, 15, 16, 17, 18, 19, 20] of first-generation (i.e., older) and second-generation[21, 22, 23] (i.e., recent) potential models. The latter fit the nucleon-nucleon scattering data very well; the best of them can be considered as alternative phase-shift analyses. This “bare-deuteron” density is folded with the sum of proton and neutron densities, and a spline fit is performed on the result. The neutron density is taken to be that of a dipole form factor multiplied by $\lambda q^2$, with $\lambda$ adjusted to fit the observed neutron mean-square charge radius: $-0.114$ fm$^2$. Finally, double and triple integrals are performed using the spline-fitted folded density (viz., the $\rho$’s in Eq. (5)).

The results are given in Table 1. We summarize the second-generation results for the deuteron as

$$I_{\text{REL}} = -3.094(4) \text{ fm}^2$$

$$\langle \ln(2\alpha\mu r) \rangle = -9.773(3)$$

$$\nu_{\text{FS}}^{(6)} = -3.40(1) \text{ kHz}.$$
Table 1: Deuteron finite-size corrections of order \((Z\alpha)^6\) for various potential models. The mean-square radius of each potential model is \(\langle r^2 \rangle\), the logarithmic radius is defined by \(\langle \ln(2\alpha \mu r) \rangle\), the relativistic density correlation is labelled \(I_{\text{REL}}\), and the corresponding deuteron 2S-1S finite-size frequency shift is \(\nu_{\text{FS}}^{(6)}\). The corresponding proton case is considered last using an exponential charge distribution. Both shifts are repulsive.

| Potential Model         | \(\langle r^2 \rangle\) (fm²) | \(\langle \ln(2\alpha \mu r) \rangle\) | \(I_{\text{REL}}\) (fm²) | \(\nu_{\text{FS}}^{(6)}\) (kHz) |
|-------------------------|-------------------------------|----------------------------------------|---------------------------|---------------------------------|
| **Second-Generation Potentials** |                               |                                        |                           |                                 |
| Argonne V₁₈             | 4.507                         | -9.770                                 | -3.091                    | -3.41                           |
| Reid Soft Core (93)     | 4.505                         | -9.771                                 | -3.095                    | -3.41                           |
| Nijmegen (loc-rel)      | 4.507                         | -9.771                                 | -3.091                    | -3.41                           |
| Nijmegen (loc-nr)       | 4.498                         | -9.773                                 | -3.090                    | -3.41                           |
| Nijmegen (nl-rel)       | 4.496                         | -9.773                                 | -3.096                    | -3.40                           |
| Nijmegen (nl-nr)        | 4.494                         | -9.776                                 | -3.094                    | -3.40                           |
| Nijmegen (full-rel)     | 4.483                         | -9.771                                 | -3.098                    | -3.39                           |
| **First-Generation Potentials** |                               |                                        |                           |                                 |
| Bonn (CS)               | 4.505                         | -9.772                                 | -3.099                    | -3.41                           |
| Argonne V₁₄             | 4.556                         | -9.762                                 | -3.108                    | -3.45                           |
| Nijmegen (78)           | 4.579                         | -9.757                                 | -3.111                    | -3.46                           |
| Super Soft Core (C)     | 4.595                         | -9.755                                 | -3.116                    | -3.48                           |
| de Tourreil-Rouben-Sprung | 4.530                     | -9.766                                 | -3.098                    | -3.43                           |
| Paris                   | 4.516                         | -9.768                                 | -3.094                    | -3.42                           |
| Reid Soft Core (68)     | 4.459                         | -9.774                                 | -3.056                    | -3.38                           |
| **Proton**              |                               |                                        |                           |                                 |
| proton                  | 0.743                         | -10.652                                | -0.473                    | -0.61                           |

We caution that these “uncertainties” are merely spreads in the potential-model results. Changing various aspects of the models that we have used (including nucleon radii) could produce larger changes than these uncertainties.

As an example of this caveat we note that the small Darwin-Foldy relativistic correction to the proton and deuteron charge densities have not been included in our model. This is easily done by adding 0.0332 fm² to the \(\langle r^2 \rangle\) of the proton (and hence to the deuteron). Consequently, the effect cancels\[^3\] in the isotopic difference. This addition modifies the proton charge radius to 0.881 fm, which increases \(\nu_{\text{FS}}^{(6)}\) by 0.03 kHz in both cases, largely by increasing \(\langle r^2 \rangle\) rather than by changing \(I_{\text{REL}}\) or \(\langle \ln(2\alpha \mu r) \rangle\).
Finally, we consider the $(Z\alpha)^5$ (second) term in Eq. (1). This is very similar in structure to the Coulomb-retardation part of the nuclear-polarization correction \[^{[1]}\], which can be written in the form

$$\Delta E_n = -\frac{\pi}{3} \alpha^2 m_e |\phi_n(0)|^2 \left[ \int d^3x \int d^3y |x - y|^3 \langle 0|\rho^\dagger(x)\rho(y)|0 \rangle - Z^2 \langle r^3 \rangle_{(2)} \right], \quad (7)$$

where the functions $\rho(x)$ and $\rho(y)$ in the correlation function $\langle 0|\rho^\dagger(x)\rho(y)|0 \rangle$ are nuclear charge operators. Ignoring the difference between $m_e$ and $\mu$ (which is of recoil order), the last term in Eq. (7) exactly cancels the second term in Eq. (1), leaving only the correlation function. That is, the separation of the nuclear Compton amplitude (which determines many of the nuclear-structure-dependent atomic corrections) into nuclear-elastic and nuclear-inelastic parts is somewhat artificial for this particular term.

The correlation function in Eq. (7) vanishes for certain (special) cases of interest to us. For the deuteron case the correlation function generates two small terms from the finite sizes of the proton (2.44 fm$^3 \rightarrow 0.032$ kHz) and the neutron (−1.58 fm$^3 \rightarrow −0.020$ kHz), which largely cancel and leave a very small residue: 0.012 kHz. Both terms vanish in the point-nucleon limit because $(\sum_i e_i)^2 \equiv \sum_i e_i^2$, where $e_i$ counts the charge of the $i$th nucleon. We note that the same cancellation takes place if we evaluate the proton correlation function in the naive, nonrelativistic, pointlike quark model (where mutatis mutandis $e_i$ counts the quark charges). In this case the individual cancelling quantities are only 0.03 kHz in size.

Table 2: Contributions in kHz to the higher-order deuteron and proton finite-size frequency shifts for the 2S-1S transition, together with their order in $(Z\alpha)$, differences between the deuteron and proton, and grand totals. Negative contributions are repulsive. For comparison the Coulomb-retardation nuclear-polarization correction, $\nu_{\text{ret}}^{\text{pol}}$, is listed also, but is not included in totals.

| Order       | $\nu_{\text{ret}}^{\text{pol}}$ | $(Z\alpha)^5$ | $(Z\alpha)^6$ | Total    |
|-------------|-------------------------------|--------------|--------------|---------|
| deuteron    | -0.48                         | 0.49         | -3.40        | -2.91   |
| proton      | -0.03                         | 0.03         | -0.61        | -0.58   |
| Isotope Shift| 0.46                          | -2.79        | -2.33        |        |

These results are displayed in Table 2, where the finite-size Coulomb corrections are listed on the right, while the Coulomb-retardation contributions to the nuclear-polarization correction are listed (for comparison only) on the left (they are not included in the totals). The cancellations are evident.
In summary, we have computed the Coulomb nuclear-finite-size corrections of orders \((Z\alpha)^5\) and \((Z\alpha)^6\) to the energy levels of hydrogenic atoms. The relatively small \((Z\alpha)^5\) term largely cancels the previously-calculated Coulomb-retardation term to the nuclear-polarization corrections for the deuteron and proton. The \((Z\alpha)^6\) contribution is larger because of a very large logarithm and because its relativistic origin precludes the need for the very small nonrelativistic factors of \((m_eR \sim \frac{1}{200})\). The net higher-order Coulomb nuclear-finite-size corrections are \(-2.91\) kHz for deuterium and \(-0.58\) kHz for the proton.

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