Eur. Phys. J. D **23**, 51–56 (2003)
DOI: 10.1140/epjd/e2003-00018-8

**THE EUROPEAN PHYSICAL JOURNAL D**

# Nuclear size correction to the hyperfine splitting in low-Z hydrogen-like atoms

A.V. Volotka[1,2], V.M. Shabaev[1,2], G. Plunien[3,a], and G. Soff[3]

[1] Department of Physics, St. Petersburg State University, Oulianovskaya 1, Petrodvorets, St. Petersburg 198504, Russia
[2] Max-Planck-Institut für Physik Komplexer Systeme, Nöthnitzer Str. 38, 01187 Dresden, Germany
[3] Institut für Theoretische Physik, TU Dresden, Mommsenstraße 13, 01062 Dresden, Germany

Received 18 March 2002 / Received in final form 14 November 2002
Published online 28 January 2003 – 

**Abstract.** The finite nuclear size effect on the hyperfine splitting of low-$Z$ hydrogen-like atoms is studied in the external field approximation. A simple non-relativistic formula is proposed which expresses the nuclear size correction to the hyperfine splitting in terms of moments of the nuclear charge and magnetization distribution. The numerical results obtained *via* this formula are compared with corresponding results derived by means of the Zemach formula. A relativistic formula for the nuclear size correction to the hyperfine splitting is also derived.

**PACS.** 31.30.Jv Relativistic and quantum electrodynamic effects in atoms and molecules – 31.30.Gs Hyperfine interactions and isotope effects, Jahn-Teller effect

## 1 Introduction

At present, the experimental value of the ground state hyperfine splitting in hydrogen is known with a relative accuracy of about $10^{-13}$ [1,2]. This accuracy is by seven orders of magnitude higher than the accuracy of the corresponding theoretical prediction [3,4]. The theoretical uncertainty is mainly determined by the uncertainty of the leading nuclear size correction. For $s$ states, this correction is generally evaluated by means of the Zemach formula [5]

$$\Delta E_{\rm NS} = \Delta E_0 \Big( -2\alpha Z m \int {\rm d}^3 r\, {\rm d}^3 r'\ \rho_{\rm e}(\mathbf{r}) \rho_{\rm m}(\mathbf{r}') |\mathbf{r}-\mathbf{r}'| \Big) . \tag{1}$$

Here $\rho_{\rm e}(\mathbf{r})$ and $\rho_{\rm m}(\mathbf{r})$ denote the nuclear charge and magnetization distribution densities normalized to

$$\int {\rm d}^3 r\ \rho_{\rm e}(\mathbf{r}) = \int {\rm d}^3 r\ \rho_{\rm m}(\mathbf{r})\ = 1 \tag{2}$$

and $\Delta E_0$ is the non-relativistic hyperfine splitting energy. Formula (1) can be used to calculate the nuclear size correction in non-relativistic external field approximation for any given model of the nuclear charge and magnetization distribution [3,4,6,7]. It would be desirable, however, to have a formula at hand which expresses the $\Delta E_{\rm NS}$ correction directly in terms of moments of the nuclear charge and magnetization distribution. In the present paper we derive a formula which achieves this goal. In the external field approximation, the corresponding relativistic formula is also derived.

It is well-known (see, *e.g.*, Ref. [3]) that the Zemach correction cancels in a specific difference $D_{n1} = n^3 \Delta E(ns) - \Delta E(1s)$, where $\Delta E(ns)$ is the hyperfine splitting of the $ns$ state. For $n = 2$, this difference is known experimentally for hydrogen [8], deuterium [9], and the $^3{\rm He}^+$ ion [10] and may be calculated with a high accuracy [3,4]. Significant progress in improving the theoretical accuracy of $D_{21}$ has been made recently by evaluating the higher-order corrections to the one-loop self-energy contribution [11] and to the one-loop vacuum-polarization contribution [4,12]. At present, one of the major sources for the theoretical uncertainty of $D_{21}$ is due to the relativistic correction to the Zemach formula. In references [3,4], this correction has been evaluated to lowest order in $\alpha Z$ and $mR_{\rm E/M}$, where $R_{\rm E/M}$ denotes the nuclear electric/magnetic radius, respectively. A dominant nuclear contribution to $D_{21}$ results from the $(\alpha Z)^2$ correction, which has been evaluated in references [3,4] by taking into account the relativistic correction to the Schrödinger wave function at the nucleus. In the present paper we rederive this correction in a more systematic way.

Relativistic and Heaviside units, where $\hbar = c = 1$ and $\alpha = e^2/(4\pi)$, are used throughout the paper.

## 2 The first-order hyperfine splitting

The interaction of the electron with the magnetic field induced by a non-zero nuclear magnetic moment leads to the

[a] e-mail: plunien@physik.tu-dresden.de

hyperfine splitting of the atomic levels. In the point-dipole approximation this interaction is given by the Fermi-Breit operator

$$H_\mu = \frac{|e|}{4\pi}\frac{(\boldsymbol{\alpha}\cdot[\boldsymbol{\mu}\times\mathbf{r}])}{r^3}\,, \tag{3}$$

where $\boldsymbol{\mu}$ is the nuclear magnetic moment operator and $\boldsymbol{\alpha}$ is the vector of the Dirac matrices. To evaluate the hyperfine splitting in a hydrogen-like atom to first order, we have to average the Fermi-Breit operator with unperturbed wave functions of the atomic system. In the case of a point nucleus, this yields [13]

$$\varDelta E = \frac{|e|}{4\pi}\frac{\mu}{I}\frac{\kappa}{j(j+1)}\frac{(\alpha Z)^3[2\kappa(\gamma+n_r)-N]m^2}{N^4\gamma(4\gamma^2-1)} \times[F(F+1)-I(I+1)-j(j+1)]\,, \tag{4}$$

where $F$ is the total angular momentum of the atom, $I$ and $j$ are the nuclear and electronic angular momenta, respectively, $n_r = n-|\kappa|$ is the radial quantum number, $n$ is the principal quantum number, $\kappa = (-1)^{j+l+1/2}(j+1/2)$ is the relativistic angular momentum quantum number, $l = j \pm 1/2$ determines the parity of the state, $\gamma = \sqrt{\kappa^2-(\alpha Z)^2}$, $N = \sqrt{n_r^2+2n_r\gamma+\kappa^2}$, and $m$ is the electron mass. In the next sections we will consider the nuclear size corrections to this splitting. We will assume the nuclear charge and magnetization distributions to be spherically symmetric, *i.e.* $\rho_{\mathrm{e}}(\mathbf{r}) = \rho_{\mathrm{e}}(r)$ and $\rho_{\mathrm{m}}(\mathbf{r}) = \rho_{\mathrm{m}}(r)$.

## 3 Nuclear charge distribution correction

For low-$Z$ hydrogen-like atoms, the nuclear charge distribution correction to the hyperfine splitting can be evaluated by perturbation theory,

$$\varDelta E_{\text{ext.ch.}} = 2\sum_N^{\varepsilon_N\neq\varepsilon_A}\frac{\langle A|\delta V_{\text{ch}}|N\rangle\langle N|H_\mu|A\rangle}{\varepsilon_A-\varepsilon_N}\,, \tag{5}$$

where $|A\rangle$ and $|N\rangle$ are the states of the total atomic system (electron plus nucleus), $\delta V_{\text{ch}}$ is the difference between the potentials of an extended and a point-charge nucleus, respectively, $\varepsilon_A$ and $\varepsilon_N$ denote the Dirac-Coulomb energies. Taking into account that $\delta V_{\text{ch}}$ is a spherically symmetric potential, we can easily integrate over the angles. As a result of this integration, we have

$$\varDelta E_{\text{ext.ch.}} = \frac{|e|}{4\pi}\frac{\mu}{I}[F(F+1)-I(I+1)-j(j+1)]\frac{\kappa}{j(j+1)} \times\sum_{n'}^{n'\neq n}\frac{\langle n\kappa|\delta V_{\text{ch}}|n'\kappa\rangle\langle n'\kappa|\frac{\sigma_x}{r^2}|n\kappa\rangle}{\varepsilon_{n\kappa}-\varepsilon_{n'\kappa}}\,, \tag{6}$$

where the two-component vector $|n\kappa\rangle$ is defined by

$$|n\kappa\rangle = \begin{pmatrix} rg_{n\kappa}(r) \\ rf_{n\kappa}(r)\end{pmatrix}$$

with $g_{n\kappa}$ and $f_{n\kappa}$ being the upper and lower radial components of the Dirac wave function as defined in reference [14]. $\sigma_x$, $\sigma_y$, $\sigma_z$ are the Pauli matrices acting in the space of the two-component vectors and the scalar product of the two-component vectors is defined by

$$\langle a|b\rangle = \int_0^\infty \mathrm{d}r\; r^2(g_a g_b + f_a f_b)\,. \tag{7}$$

The sum

$$|\xi\rangle = \sum_{n'}^{n'\neq n}\frac{|n'\kappa\rangle\langle n'\kappa|\frac{\sigma_x}{r^2}|n\kappa\rangle}{\varepsilon_{n\kappa}-\varepsilon_{n'\kappa}} \tag{8}$$

can be calculated by employing the generalized virial relations for the Dirac equation [15]. Such a calculation yields [16]

$$\begin{aligned}|\xi\rangle = &\frac{1}{4(\alpha Z)^2+(1-4\kappa^2)} \\ &\times\Big\{2\alpha Z\frac{\sigma_x}{r}+4\alpha Z\kappa i\frac{\sigma_y}{r}+(1-4\kappa^2)\frac{\sigma_z}{r}-\frac{2(\alpha Z)^3\kappa m}{N^3\gamma} \\ &-\frac{1-4\kappa^2}{\kappa}(\varepsilon_{n\kappa}i\sigma_y+m\sigma_x)\Big\}|n\kappa\rangle \\ &-\frac{2\alpha Z(2\varepsilon_{n\kappa}-m/\kappa)}{4(\alpha Z)^2+(1-4\kappa^2)}\frac{\mathrm{d}}{\mathrm{d}\kappa}|n\kappa\rangle.\end{aligned} \tag{9}$$

When evaluating matrix elements with $\delta V_{\text{ch}}(r)$, which deviates from zero only inside the nucleus, the radial function $|\xi\rangle$ as well as $|n\kappa\rangle$ can be approximated by the lowest order term of the series expansion in powers of $r$. (In particular, it means that the last term in equation (9) can be omitted.) Accordingly, we have to evaluate the integral

$$I = \int \mathrm{d}^3r\; r^\beta\delta V_{\text{ch}}\,. \tag{10}$$

Employing the identity

$$r^\beta = \frac{1}{(\beta+2)(\beta+3)}\varDelta r^{\beta+2}\,, \tag{11}$$

where $\varDelta$ is the Laplacian, and integrating by parts, we obtain

$$\begin{aligned}I &= \int \mathrm{d}^3r\;\frac{\varDelta r^{\beta+2}}{(\beta+2)(\beta+3)}\delta V_{\text{ch}} \\ &= \int \mathrm{d}^3r\;\frac{r^{\beta+2}}{(\beta+2)(\beta+3)}\varDelta(\delta V_{\text{ch}}).\end{aligned} \tag{12}$$

By means of the Poisson equation

$$\varDelta(\delta V_{\text{ch}}(r)) = 4\pi\alpha Z[\rho_{\mathrm{e}}(r)-\delta(\mathbf{r})]\,, \tag{13}$$

we derive

$$I = 4\pi\alpha Z\frac{\langle r^{\beta+2}\rangle_{\mathrm{e}}}{(\beta+2)(\beta+3)}\,, \tag{14}$$

**Table 1.** The nuclear charge distribution correction $\delta_{\rm e}$, in %, for the $1s$ state, calculated by means of formulas (15, 17, 18, 20). For comparison, the results of a more accurate numerical calculation [17] are given in the seventh column. The values for $\langle r^2\rangle_{\rm e}^{1/2}$ are taken from [18–20].

| $Z$ | $\langle r^2\rangle_{\rm e}^{1/2}$ [fm] | Eq. (18) | Eq. (17) | Eq. (15) | Eq. (20) | Ref. [17] |
|---|---|---|---|---|---|---|
| 1 | 0.862 | 0.00315 | 0.00315 | 0.00315 | 0.00315 | 0.00315 |
| 5 | 2.452 | 0.0449 | 0.0456 | 0.0456 | 0.0455 | 0.0455 |
| 10 | 2.967 | 0.109 | 0.115 | 0.115 | 0.114 | 0.114 |
| 15 | 3.190 | 0.175 | 0.197 | 0.198 | 0.193 | 0.194 |
| 20 | 3.495 | 0.256 | 0.309 | 0.316 | 0.301 | 0.306 |

where $\langle r^\beta\rangle_{\rm e} = \int {\rm d}^3r\ r^\beta \rho_{\rm e}(r)$. Thus the nuclear charge distribution correction (6) takes the form

$$\begin{aligned}\Delta E_{\rm ext.ch.} = &\frac{|e|}{4\pi}\frac{\mu}{I}[F(F+1)-I(I+1)-j(j+1)] \\ &\times \frac{\kappa}{j(j+1)}\frac{\Gamma(2\gamma+n_r+1)}{\Gamma^2(2\gamma+1)n_r!} \\ &\times \Big\{2\alpha Z\sqrt{m^2-\varepsilon_{n\kappa}^2}(n_r^2-(N-\kappa)^2) \\ &+(1-4\kappa^2)[\varepsilon_{n\kappa}(n_r^2+(N-\kappa)^2)-2n_r m(N-\kappa)]\Big\} \\ &\times\left(\frac{2\alpha Z}{N}\right)^{2\gamma+1}\frac{\alpha Z m^{2\gamma}}{(4(\alpha Z)^2+(1-4\kappa^2))4N(N-\kappa)}\frac{\langle r^{2\gamma-1}\rangle_{\rm e}}{\gamma(2\gamma-1)}, \quad (15)\end{aligned}$$

where $\Gamma(x)$ is the gamma function. For low-$Z$ atoms it is convenient to express this correction in terms of $\delta_{\rm e}$ defined by

$$\Delta E_{\rm ext.ch.} = -\Delta E_0 \delta_{\rm e}\,, \quad (16)$$

where $\Delta E_0$ denotes the non-relativistic hyperfine splitting energy. Keeping the two lowest-order terms in $\alpha Z$, equation (15) yields for the $s$ states

$$\begin{aligned}\delta_{\rm e}^{(s)} = 2\alpha Z m\langle r\rangle_{\rm e}\Bigg\{&1+(\alpha Z)^2\Big[2\psi(3)-\psi(n+1) \\ &-\log\left(\frac{2\alpha Z}{n}\right)-\frac{\langle r\log(mr)\rangle_{\rm e}}{\langle r\rangle_{\rm e}}+\frac{8n-9}{4n^2}+\frac{11}{4}\Big]\Bigg\}, \quad (17)\end{aligned}$$

where $\psi(x) = \frac{\rm d}{{\rm d}x}\log\Gamma(x)$. The non-relativistic limit is given by

$$\delta_{\rm e}^{(s){\rm nr}} = 2\alpha Z m\langle r\rangle_{\rm e}\,. \quad (18)$$

For the $p_{\frac{1}{2}}$ states, one easily finds in the non-relativistic limit

$$\delta_{\rm e}^{(p_{\frac{1}{2}}){\rm nr}} = \frac{3}{2}(\alpha Z)^3 m\langle r\rangle_{\rm e}\frac{n^2-1}{n^2}\cdot \quad (19)$$

Formulas (18, 19) coincide with the related expressions derived in [17] for the case of a homogeneously charged sphere, while the relativistic $n$-independent term in formula (17) differs from the corresponding term that can be derived from the formulas presented in [17]. Since, for the sphere model, the approach developed in [17] provides a more accurate evaluation of the nuclear size correction than the perturbation theory considered here, formula (17) can be improved by replacing the relativistic $n$-independent term with the corresponding term derived from [17]. As a result, we obtain

$$\begin{aligned}\delta_{\rm e}^{(s)} = 2\alpha Z m\langle r\rangle_{\rm e}\Bigg\{&1+(\alpha Z)^2\Big[2\psi(3)-\psi(n+1) \\ &-\log\left(\frac{2\alpha Z}{n}\right)-\frac{\langle r\log(mr)\rangle_{\rm e}}{\langle r\rangle_{\rm e}}+\frac{8n-9}{4n^2}+\frac{839}{750}\Big]\Bigg\}\cdot \quad (20)\end{aligned}$$

Formulas (17, 20) differ only by the last constant term.

In Tables 1, 2, and 3 we present numerical values of $\delta_{\rm e}$ as calculated according to equations (15–20) and compare them with the results of a more accurate numerical evaluation [17]. All the calculations are performed for the

**Table 2.** The nuclear charge distribution correction $\delta_{\rm e}$, in %, for the $2s$ state, calculated by means of formulas (15, 17, 18, 20). For comparison, the results of a more accurate numerical calculation [17] are given in the sixth column. The values for $\langle r^2\rangle_{\rm e}^{1/2}$ are the same as in Table 1.

| $Z$ | Eq. (18) | Eq. (17) | Eq. (15) | Eq. (20) | Ref. [17] |
|---|---|---|---|---|---|
| 1 | 0.00315 | 0.00315 | 0.00315 | 0.00315 | 0.00315 |
| 5 | 0.0449 | 0.0456 | 0.0456 | 0.0455 | 0.0455 |
| 10 | 0.109 | 0.115 | 0.116 | 0.114 | 0.114 |
| 15 | 0.175 | 0.198 | 0.200 | 0.195 | 0.197 |
| 20 | 0.256 | 0.314 | 0.322 | 0.305 | 0.311 |

**Table 3.** The nuclear charge distribution correction $\delta_{\rm e}$, in %, for the $2p_{\frac{1}{2}}$ state, calculated by means of formulas (15, 19). For comparison, the results of a more accurate numerical calculation [17] are given in the fourth column. The values for $\langle r^2\rangle_{\rm e}^{1/2}$ are the same as in Table 1. The symbol $[-n]$ means $\times 10^{-n}$.

| $Z$ | Eq. (19) | Eq. (15) | Ref. [17] |
|---|---|---|---|
| 1 | 0.945[−7] | 0.945[−7] | 0.945[−7] |
| 5 | 0.336[−4] | 0.342[−4] | 0.342[−4] |
| 10 | 0.325[−3] | 0.347[−3] | 0.344[−3] |
| 15 | 0.118[−2] | 0.136[−2] | 0.133[−2] |
| 20 | 0.306[−2] | 0.390[−2] | 0.377[−2] |

**Table 4.** The nuclear magnetization distribution correction $\delta_{\rm m}$, in %, for the 1$s$ and 2$s$ states, as calculated *via* formulas (26, 27). The sphere model is employed for the nuclear charge and magnetization distributions. For comparison, the results of a more accurate numerical calculation [17] are given in the fifth and eighth columns. The values for $\langle r^2\rangle_{\rm e}^{1/2}$ are taken from [18–20].

| $Z$ | $\langle r^2\rangle_{\rm e/m}^{1/2}$ [fm] | 1$s$, Eq. (27) | 1$s$, Eq. (26) | 1$s$, [17] | 2$s$, Eq. (27) | 2$s$, Eq. (26) | 2$s$, [17] |
|---|---|---|---|---|---|---|---|
| 1 | 0.862 | 0.00117 | 0.00117 | 0.00117 | 0.00117 | 0.00117 | 0.00117 |
| 5 | 2.452 | 0.0167 | 0.0169 | 0.0169 | 0.0167 | 0.0169 | 0.0169 |
| 10 | 2.967 | 0.0403 | 0.0419 | 0.0420 | 0.0403 | 0.0421 | 0.0422 |
| 15 | 3.190 | 0.0650 | 0.0705 | 0.0709 | 0.0650 | 0.0712 | 0.0716 |
| 20 | 3.495 | 0.0950 | 0.108 | 0.110 | 0.0950 | 0.110 | 0.112 |

homogeneously charged sphere model of the nuclear charge distribution.

## 4 Nuclear magnetization distribution correction

For low-$Z$ atoms the nuclear magnetization distribution correction can be written as

$$\Delta E_{\rm ext.mag.} = -\Delta E \int {\rm d}^3 r\; K(r)\rho_{\rm m}(r)\,, \qquad (21)$$

where $\Delta E$ is given by equation (4), $\rho_{\rm m}(r)$ is the nuclear magnetization distribution density, and $K(r)$ is defined by

$$K(r) = \frac{\displaystyle\int_0^r {\rm d}r'\; f_{n\kappa}(r')g_{n\kappa}(r')}{\displaystyle\int_0^\infty {\rm d}r'\; f_{n\kappa}(r')g_{n\kappa}(r')}\cdot \qquad (22)$$

In order to derive an analytical expression for this correction, we will employ the sphere model for the nuclear charge distribution, with a radius $R_0 = \sqrt{5/3}\langle r^2\rangle_{\rm e}^{1/2}$, keeping the lowest-order term in $mR_0$ and the two lowest-order terms in $\alpha Z$. For the $s$ states, the function $K(r)$ is given by [17]

$$\begin{aligned} K^{(s)}(r) &= \alpha Z m R_0\left(\frac{r^2}{R_0^2} - \frac{r^4}{10R_0^4}\right) + (\alpha Z)^3 m R_0 \\ &\times\Biggl\{\Biggl[2\Psi(3) - \Psi(n+1) - \log\left(\frac{2\alpha Z m R_0}{n}\right) \\ &- \frac{112n^2 - 30n + 25}{60n^2}\Biggr]\left(\frac{r^2}{R_0^2} - \frac{r^4}{10R_0^4}\right) \\ &- \frac{1}{5}\left(\frac{3r^4}{2R_0^4} - \frac{19r^6}{42R_0^6} + \frac{19r^8}{360R_0^8} - \frac{2}{825}\frac{r^{10}}{R_0^{10}}\right)\Biggr\}. \end{aligned} \qquad (23)$$

Although equation (23) holds strictly only for $r \le R_0$, it yields a reasonably good approximation for $K^{(s)}(r)$ in the region $R_0 < r < 2R_0$ as well. Introducing $\delta_{\rm m}$ *via*

$$\Delta E_{\rm ext.mag.} = -\Delta E_0 \delta_{\rm m}, \qquad (24)$$

we easily find

$$\delta_{\rm m} = \frac{\Delta E}{\Delta E_0}\int {\rm d}^3 r\; K(r)\rho_{\rm m}(r). \qquad (25)$$

Substituting (23) into (25), we obtain to first order in $mR_0$ and to two lowest orders in $\alpha Z$

$$\begin{aligned} \delta_{\rm m}^{(s)} &= \alpha Z m R_0\left(\frac{\langle r^2\rangle_{\rm m}}{R_0^2} - \frac{\langle r^4\rangle_{\rm m}}{10R_0^4}\right) + (\alpha Z)^3 m R_0 \\ &\times\Biggl\{\Biggl[2\Psi(3) - \Psi(n+1) - \log\left(\frac{2\alpha Z m R_0}{n}\right) \\ &+ \frac{8n-9}{4n^2} - \frac{1}{30}\Biggr]\left(\frac{\langle r^2\rangle_{\rm m}}{R_0^2} - \frac{\langle r^4\rangle_{\rm m}}{10R_0^4}\right) \\ &- \frac{1}{5}\left(\frac{3\langle r^4\rangle_{\rm m}}{2R_0^4} - \frac{19\langle r^6\rangle_{\rm m}}{42R_0^6} + \frac{19\langle r^8\rangle_{\rm m}}{360R_0^8} - \frac{2}{825}\frac{\langle r^{10}\rangle_{\rm m}}{R_0^{10}}\right)\Biggr\}. \end{aligned} \qquad (26)$$

In the non-relativistic approximation, we have

$$\delta_{\rm m}^{(s){\rm nr}} = \alpha Z m R_0\left(\frac{\langle r^2\rangle_{\rm m}}{R_0^2} - \frac{1}{10}\frac{\langle r^4\rangle_{\rm m}}{R_0^4}\right)\cdot \qquad (27)$$

In Table 4 we present numerical results for $\delta_{\rm m}$ and compare them with the more accurate numerical results obtained in [17]. The sphere model has been used for the nuclear charge and magnetization distributions. As one can see from the table, formula (26) properly accounts for the relativistic effects.

Formulas (26, 27) are derived for the homogeneously charged sphere model of the nuclear charge distribution. However, they also yield sufficiently accurate results for other models of the nuclear charge distribution (with $R_0 = \sqrt{5/3}\langle r^2\rangle_{\rm e}^{1/2}$), which are close enough to the homogeneously charged sphere model.

## 5 Discussion

According to the formulas derived above, the total finite nuclear size correction to the hyperfine splitting of an $ns$ state in a low-$Z$ hydrogen-like atom is given by

$$\Delta E_{\rm NS} = \Delta E_{\rm ext.ch.} + \Delta E_{\rm ext.mag.} = -\Delta E_0(\delta_{\rm e} + \delta_{\rm m}), \qquad (28)$$

**Table 5.** The total nuclear size correction $\delta_\mathrm{e} + \delta_\mathrm{m}$, expressed in %, for the $s$ states, calculated by means of formula (30). The sphere model is used for the nuclear charge distribution together with four different models for the nuclear magnetization distribution as described in the text. For comparison, the corresponding results derived from the Zemach formula [5] are presented as well. The values for $\langle r^2\rangle_\mathrm{e}^{1/2}$ are taken from [18–20]. The values for $\langle r^2\rangle_\mathrm{m}^{1/2}$ are assumed to be equal to the corresponding values for $\langle r^2\rangle_\mathrm{e}^{1/2}$.

| $Z$ | $\langle r^2\rangle_\mathrm{e/m}^{1/2}$ [fm] | S | S [5] | SS | SS [5] | E | E [5] | G | G [5] |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 0.862 | 0.00433 | 0.00433 | 0.00434 | 0.00434 | 0.00423 | 0.00425 | 0.00429 | 0.00429 |
| 2 | 1.844 | 0.0185 | 0.0185 | 0.0186 | 0.0186 | 0.0181 | 0.0182 | 0.0184 | 0.0184 |
| 3 | 2.39 | 0.0360 | 0.0360 | 0.0361 | 0.0361 | 0.0352 | 0.0353 | 0.0357 | 0.0357 |
| 5 | 2.452 | 0.0615 | 0.0615 | 0.0617 | 0.0617 | 0.0601 | 0.0604 | 0.0610 | 0.0610 |
| 10 | 2.967 | 0.149 | 0.149 | 0.149 | 0.149 | 0.145 | 0.146 | 0.148 | 0.148 |

where

$$\delta_\mathrm{e}^{(s)} + \delta_\mathrm{m}^{(s)} = (\delta_\mathrm{e}^{(s)\mathrm{nr}} + \delta_\mathrm{m}^{(s)\mathrm{nr}})\Bigg\{1 + (\alpha Z)^2\Bigg[2\Psi(3) - \Psi(n+1) - \log\left(\frac{2\alpha Z}{n}\right) + \frac{8n-9}{4n^2}\Bigg]\Bigg\} - \delta_\mathrm{m}^{(s)\mathrm{nr}}(\alpha Z)^2\left(\log(mR_0) + \frac{1}{30}\right) - \delta_\mathrm{e}^{(s)\mathrm{nr}}(\alpha Z)^2\left(\frac{\langle r\log(mr)\rangle_\mathrm{e}}{\langle r\rangle_\mathrm{e}} - \frac{839}{750}\right) - \frac{(\alpha Z)^3 mR_0}{5}\left(\frac{3\langle r^4\rangle_\mathrm{m}}{2R_0^4} - \frac{19\langle r^6\rangle_\mathrm{m}}{42R_0^6} + \frac{19\langle r^8\rangle_\mathrm{m}}{360R_0^8} - \frac{2}{825}\frac{\langle r^{10}\rangle_\mathrm{m}}{R_0^{10}}\right). \quad (29)$$

The corresponding non-relativistic approximation is given by

$$\delta_\mathrm{e}^{(s)\mathrm{nr}} + \delta_\mathrm{m}^{(s)\mathrm{nr}} = 2\alpha Zm\langle r\rangle_\mathrm{e} + \alpha ZmR_0\left(\frac{\langle r^2\rangle_\mathrm{m}}{R_0^2} - \frac{1}{10}\frac{\langle r^4\rangle_\mathrm{m}}{R_0^4}\right). \quad (30)$$

To compare this non-relativistic formula with the Zemach expression, let us consider the following models for the nuclear magnetization distribution:

1. the sphere model (S model)

$$\rho_\mathrm{m}(r) = \frac{\theta(R_0 - r)}{\frac{4}{3}\pi R_0^3}, \quad (31)$$

2. the spherical shell model (SS model)

$$\rho_\mathrm{m}(r) = \frac{\delta(R_0 - r)}{4\pi R_0^2}, \quad (32)$$

3. an exponential distribution (E model)

$$\rho_\mathrm{m}(r) = \frac{\Lambda^3}{8\pi}\mathrm{e}^{-\Lambda r}, \quad (33)$$

4. a Gaussian distribution (G model)

$$\rho_\mathrm{m}(r) = \frac{\Lambda^{\frac{3}{2}}}{2\pi\Gamma(\frac{3}{2})}\mathrm{e}^{-\Lambda r^2}. \quad (34)$$

In Table 5 we present the non-relativistic values for the total nuclear size correction employing the sphere model of the nuclear charge distribution together with various models of the nuclear magnetization distributions as calculated by means of equation (30). For comparison, the results obtained by the Zemach formula are also presented in the table. As one can see from the table, the results derived by formula (30) are in very good agreement with the Zemach values. It can be shown that a slight difference between the Zemach results and our non-relativistic results, as it appears, *e.g.*, for the E model, is determined by the integral

$$\Delta\delta_\mathrm{m}^{(s)\mathrm{nr}} = 8\pi\frac{\alpha Z}{R_0^3}\int_{R_0}^{\infty}\mathrm{d}r\,\rho_\mathrm{m}(r)r \times\left(\frac{1}{5}R_0^5 - \frac{3}{4}rR_0^4 + r^2R_0^3 - \frac{1}{2}r^3R_0^2 + \frac{1}{20}r^5\right). \quad (35)$$

Performing similar calculations employing other models for the nuclear charge distribution (with $R_0 = \sqrt{5/3}\langle r^2\rangle_\mathrm{e}^{1/2}$) and comparing the corresponding results with the Zemach ones, again a good agreement is obtained for models of the nuclear charge distribution that are close to the sphere model. In particular, it follows that for all these models the relativistic correction to the Zemach formula can be determined by equation (29) with a good accuracy.

To compare the $n$-dependent terms in formula (29) with those in references [3,4], we consider the difference

$$D_{n1}^\mathrm{NS} = n^3\Delta E_\mathrm{NS}^{(ns)} - \Delta E_\mathrm{NS}^{(1s)}. \quad (36)$$

From equation (29), we derive

$$D_{n1}^\mathrm{NS} = (\alpha Z)^2\left(\Psi(n+1) - \Psi(2) - \log n - \frac{(n-1)(n+9)}{4n^2}\right) \times\Delta E_0^{(1s)}(\delta_\mathrm{e}^{(s)\mathrm{nr}} + \delta_\mathrm{m}^{(s)\mathrm{nr}}). \quad (37)$$

Here $\Delta E_0^{(1s)}$ is the ground-state hyperfine splitting obtained from the non-relativistic theory. This expression exactly coincides with the corresponding formula derived in references [3,4]

In conclusion, we derived relativistic and non-relativistic formulas which express the nuclear size correction to the hyperfine splitting in terms of moments of the nuclear charge and magnetization distributions. Although the magnetization distribution correction has been derived employing the sphere model for the nuclear charge distribution, to a good accuracy, the formulas may also apply for other models that are close enough to the sphere model.

We thank I.I. Tupitsyn for providing us with the numerical results for the nuclear charge distribution correction obtained by a direct solution of the Dirac equation. Valuable conversations with T. Beier and S. Karshenboim are gratefully acknowledged. This work was supported in part by RFBR (Grant No. 01-02-17248), by the program "Russian Universities" (Grant No. UR.01.01.072), by DAAD, and by GSI.

## References

1. H. Hellwig, R.F.C. Vessot, M.W. Levine, P.W. Zitzewitz, D.W. Allan, D.J. Glaze, IEEE Trans. Instr. Meas. IM **19**, 200 (1970)
2. L. Essen, R.W. Donaldson, M.J. Bangham, E.G. Hope, Nature **229**, 110 (1971)
3. S.G. Karshenboim, Phys. Lett. A **225**, 97 (1997); *Hydrogen atom: Precision physics of simple atomic systems*, edited by S.G. Karshenboim *et al.* (Springer, Berlin, 2001), p. 335; e-print physics/0102085 (2001)
4. S.G. Karshenboim, V.G. Ivanov, Phys. Lett. B **524**, 259 (2002); Eur. Phys. J. D **19**, 13 (2002)
5. A.C. Zemach, Phys. Rev. **104**, 1771 (1956)
6. C.K. Iddings, P.M. Platzman, Phys. Rev. **113**, 192 (1959)
7. G.T. Bodwin, D.R. Yennie, Phys. Rev. D **37**, 498 (1988)
8. N.E. Rothery, E.A. Hessels, Phys. Rev. A **61**, 044501 (2000)
9. H.A. Reich, J.W. Heberle, P. Kush, Phys. Rev. **104**, 1585 (1956)
10. M.H. Prior, E.C. Wang, Phys. Rev. A **16**, 6 (1977)
11. V.A. Yerokhin, V.M. Shabaev, Phys. Rev. A **64**, 012506 (2001)
12. S.G. Karshenboim, V.G. Ivanov, V.M. Shabaev, Can. J. Phys. **76**, 503 (1998); JETP **90**, 59 (2000)
13. P. Pyykkö, E. Pajanne, M. Inokuti, Int. J. Quant. Chem. **7**, 785 (1973)
14. A.I. Akhiezer, V.B. Berestetsky, *Quantum Electrodynamics* (Nauka, Moscow, 1969)
15. V.M. Shabaev, J. Phys. B **24**, 4479 (1991)
16. M.B. Shabaeva, V.M. Shabaev, Phys. Rev. A **52**, 2811 (1995)
17. V.M. Shabaev, J. Phys. B **27**, 5825 (1994)
18. G.G. Simon, C. Schmidt, F. Borkowski, V.H. Walther, Nucl. Phys A **333**, 381 (1980)
19. H. de Vries, C.W. de Jager, C. de Vries, At. Data Nucl. Data Tables **36**, 3 (1987)
20. G. Fricke, C. Bernhardt, K. Heilig, L.A. Schaller, L. Schellenberg, E.B. Shera, C.W. de Jager, At. Data Nucl. Data Tab. **60**, 177 (1995)