ELECTRIC QUADRUPOLE MOMENT OF A HYDROGENLIKE ION IN $s$ AND $p_{1/2}$ STATES

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Abstract

Relativistic formulas for the electric quadrupole moment of a hydrogenlike atom, induced by the hyperfine interaction, are derived for $ns$ and $np_{1/2}$ states. Both the magnetic dipole and electric quadrupole hyperfine interactions are taken into account. The formulas are valid for ions with arbitrary nuclear charge and spin. The induced quadrupole moment is compared with the nuclear quadrupole moment for a wide range of hydrogenlike ions.

1 Introduction

In Ref. [1] it was first noted that a hydrogen atom in the triplet $s$ state has an electric quadrupole moment. This is caused by the admixture of the $d_{3/2}$ states to the $s$ state due to the hyperfine interaction between the electron and the magnetic dipole moment of the nucleus ($\text{HFI}_\mu$). In Refs. [2–4], the quadrupole moment ($\text{QM}_\mu$) of a hydrogenlike atom in the $1s$ state was calculated in the full relativistic theory:

$$Q_\mu(1s, Z, I, \mu) = \frac{2\gamma + 1}{3} \frac{\eta \mu}{Z \mu_N} Q_1,$$  

Here

$$Q_1 = \frac{1}{3} \alpha^2 m_e a^2,$$

$Z$ is the nuclear charge number, $I$ is the nuclear spin, $\alpha$ is the fine structure constant, $a$ is the Bohr radius, $m_e$ and $m_p$ are the electron and proton masses, respectively, $\mu$ is the magnetic moment of the nucleus, $\mu_N = |e|\hbar/(2m_pc)$ is the nuclear magneton, $\gamma = [1 - (\alpha Z)^2]^{1/2}$,

$$\eta = (-1)^{F-I-1/2} \frac{F(2F-1)(2F+1)}{I(I+F+1/2)(I+F+3/2)}$$

and $F$ is the total atomic angular momentum. For the $ns$ state with $F = 1$, $I = 1/2$ the corresponding calculation to the lowest order in $\alpha Z$ yields [5]:

$$Q_\mu(ns, 1, 1/2, \mu) = \frac{n^2 + 2}{3} \frac{\mu}{\mu_N} Q_1.$$  

A hydrogenlike atom has the $\text{QM}_\mu$ also in $p_{1/2}$ states, which is caused by the admixture of $p_{3/2}$ states. The relativistic theory of the $\text{QM}_\mu$ for a hydrogenlike atom in the $2p_{1/2}$ state with $F = 1$, $I = 1/2$ gives [6]:

$$Q_\mu(2p_{1/2}, Z, 1/2, \mu) = -\frac{1}{15} \frac{N-1}{2-N} (4N^3 + N^2 + 9N - 6) \frac{\mu}{Z \mu_N} Q_1.$$  

where \( N = (2 + 2\gamma)^{1/2} \).

The electric quadrupole hyperfine interaction of the electron with the nucleus (HFI\(_Q\)) can also induce a nonzero electric quadrupole moment of the atom (QM\(_Q\)), mixing the \( s \) states with the \( d \) states, and the \( p_{1/2} \) states with the \( p_{3/2} \) and \( f_{5/2} \) states. However, since for light atoms the HFI\(_Q\) is much weaker than the HFI\(_\mu\) and, in addition, it can contribute only for atoms with the nuclear spin \( I > 1/2 \), it was generally disregarded in previous calculations.

In the present paper, we derive relativistic expressions for the electric quadrupole moment of a hydrogenlike ion being in \( ns \) and \( np_{1/2} \) states. The derived formulas are valid for ions with arbitrary nuclear charge, spin, magnetic dipole and electric quadrupole moments. Both magnetic dipole and electric quadrupole hyperfine interactions are taken into account.

Relativistic and Heaviside charge units (\( \hbar = c = 1 \), \( \alpha = e^2/4\pi \)) are used in the paper, the charge of the electron is taken to be \( e < 0 \).

2 Induced quadrupole moment

The hyperfine interaction operator is given by the sum

\[
H_{\text{HFI}} = H_\mu + H_Q,
\]

where \( H_\mu \) and \( H_Q \) are the magnetic-dipole and electric-quadrupole hyperfine interaction operators, respectively. In the point-dipole approximation,

\[
H_\mu = \frac{|e|}{4\pi} (\vec{\alpha} \cdot [\vec{\mu} \times \vec{r}]) \frac{1}{r^3},
\]

and, in the point-quadrupole approximation,

\[
H_Q = -\alpha \sum_{m=-2}^{m=2} Q_{2m} \eta_{2m}^*(\vec{n}).
\]

Here the vector \( \vec{\alpha} \) incorporates the Dirac \( \alpha \) matrices, \( \vec{\mu} \) is the nuclear magnetic moment operator acting in the space of nuclear variables, \( Q_{2m} = \sum_{i=1}^{Z} r_i^2 C_{2m}(\vec{n}_i) \) is the operator of the electric quadrupole moment of the nucleus, \( \eta_{2m} = C_{2m}(\vec{n})/r^3 \) is an operator that acts on electron variables, \( \vec{n} = \vec{r}/r \), \( \vec{r} \) is the position vector of the electron, \( \vec{r}_i \) is the position vector of the \( i \)th proton in the nucleus, \( C_{lm} = \sqrt{4\pi/(2l+1)} Y_{lm} \), and \( Y_{lm} \) is a spherical harmonic. It must be stressed that the electric quadrupole interaction should be taken into account only for ions with \( I > 1/2 \). Thus the quadrupole moment of a hydrogenlike atom in the \( |A\rangle \) state, induced by the hyperfine interaction, is given by

\[
Q_\mu(A) + Q_Q(A) = 2 \sum_{N \neq E_A} \frac{\langle A|Q_{zz}|N\rangle \langle N|H_\mu + H_Q|A\rangle}{E_A - E_N}, \quad (M_{F_A} = F_A),
\]

where \( Q_{zz} = -r^2(3n_z^2 - 1) \), \( |A\rangle \) and \( |N\rangle \) are the state vectors of the total (electron plus nucleus) atomic system, \( E_A \) and \( E_N \) are the related energies.

Let us consider first the \( ns \) state. Integrating over angular variables in \( (9) \) yields

\[
Q_\mu(ns, Z, I, \mu) = \frac{2e}{15\pi} \eta \mu \langle n - 1|r^2|\xi_1(2; n, -1)\rangle,
\]

and

\[
Q_Q(ns, Z, I, Q_N) = \alpha \tau Q_N(2\langle n - 1|r^2|\xi_2(2; n, -1)\rangle + 3\langle n - 1|r^2|\xi_2(-3; n, -1)\rangle).
\]
Here $\mu = \langle II | \mu_z | II \rangle$ is the nuclear magnetic moment, $Q_N = 2\langle II | Q_{20} | II \rangle$ is the electric quadrupole moment of the nucleus,

$$
\tau = \begin{cases} 
\frac{2}{25I(2I+1)}, & F = I + 1/2, I \neq 1/2 \\
\frac{2(I-1)(2I+3)}{25I(2I+1)}, & F = I - 1/2, I \neq 1/2 \\
0, & I = 1/2 
\end{cases}.
$$

$$
| \xi_1(\kappa'; n, \kappa) \rangle \equiv \sum_{n'} \frac{(E_{n',\kappa'} \neq E_{n,\kappa}) \langle n'\kappa'| \sigma_x r^{-2} | n\kappa \rangle}{E_{n,\kappa} - E_{n',\kappa'}},
$$

$$
| \xi_2(\kappa'; n, \kappa) \rangle \equiv \sum_{n'} \frac{|n'\kappa'| \langle n'\kappa'| r^{-3} | n\kappa \rangle}{E_{n,\kappa} - E_{n',\kappa'}}.
$$

$\sigma_x$ is the Pauli matrix, the vector $| n\kappa \rangle = \left( \frac{rg_{n\kappa}}{r f_{n\kappa}} \right)$, $(\langle n\kappa | n\kappa \rangle = \int_0^\infty (g_{n\kappa}^2 + f_{n\kappa}^2) r dr = 1)$ consists of the upper and lower radial components of the Dirac wave function defined by

$$
|n\kappa m\rangle = \begin{pmatrix} g_{n\kappa}(r) \Omega_{km}(\vec{\kappa}) \\ if_{n\kappa}(r) \Omega_{-km}(\vec{\kappa}) \end{pmatrix},
$$

$\kappa = (-1)^{j+l+1}(j + 1/2)$ and $E_{n,\kappa}$ is the Dirac energy. For the point-charge nucleus, the sums $\xi_1$ and $\xi_2$, can be evaluated analytically, employing the method of generalized virial relations for the Dirac equation in a central field [7, 8]. For $\kappa \neq \pm \kappa'$ one can derive [7, 8]

$$
|\xi_1(\kappa', n\kappa)\rangle = \{[1 - (\kappa - \kappa')^2][1 - (\kappa + \kappa')^2] + 4(\alpha Z)^2\}^{-1} \times \left[ 1 - (\kappa + \kappa')^2 \left( \frac{4\alpha Z m_e}{\kappa^2 - \kappa'^2} + (\kappa' - \kappa) r^{-1} + r^{-1} \sigma_x \right) - \frac{2}{\kappa + \kappa'}(m_e \sigma_x + E_{n,\kappa}i\sigma_y) \right] + 2\alpha Z[\sigma_x r^{-1} + (\kappa + \kappa') r^{-1} i\sigma_y] |n\kappa\rangle,
$$

and [11]

$$
|\xi_2(\kappa', n\kappa)\rangle = \{[4 - (\kappa - \kappa')^2][4 - (\kappa + \kappa')^2] + 16(\alpha Z)^2\}^{-1} \left[ 2\alpha Z(\kappa^2 - \kappa'^2) \frac{1}{r^2} \right. \\
- 4\alpha Z(\kappa + \kappa') \frac{\sigma_z}{r^2} + \frac{D_1}{D_0} \frac{D_2}{D_0} \frac{D_0}{r^2} + \frac{D_2(\kappa + \kappa')}{D_0} \\
- 8\alpha Z m_e(\kappa + \kappa') \frac{i\sigma_y}{r^2} + \frac{D_1}{D_0} \frac{D_2}{D_0} \frac{D_0}{r^2} - \frac{2}{\kappa + \kappa'}(m_e \sigma_x + E_{n,\kappa}i\sigma_y) \\
+ \frac{4\alpha Z m_e D_1}{\kappa^2 - \kappa'^2 D_0} + \frac{2m_e(\kappa + \kappa') - 2E_{n,\kappa} D_2}{D_0} - \frac{16\alpha Z m_e^2(\kappa + \kappa')}{\kappa - \kappa'} \left] |n\kappa\rangle,
$$

where $\sigma_y$ and $\sigma_z$ are the Pauli matrices,

$$
D_0 = [1 - (\kappa + \kappa')^2][1 - (\kappa - \kappa')^2] + 4(\alpha Z)^2 ,
$$

$$
D_1 = 2m_e[8(\alpha Z)^2(\kappa + \kappa')^2 + (1 - (\kappa + \kappa')^2)(8 + 8(\alpha Z)^2 - 2(\kappa - \kappa')^2)] + 2E_{n,\kappa}(\kappa + \kappa') [8(\alpha Z)^2 + (1 - (\kappa + \kappa')^2)((\kappa - \kappa')^2 - 4)],
$$

$$
D_2 = 8\alpha Z m_e[4 + 4(\alpha Z)^2 - (\kappa - \kappa')^2 - (\kappa + \kappa')^2[(1 - (\kappa - \kappa')^2)] \\
+ 12\alpha Z E_{n,\kappa}(\kappa + \kappa')[(\kappa - \kappa')^2 - 2].
$$
Further calculations of expressions (10), (11) can easily be performed by using the recurrent formulas for the expectation values \( A^s = \langle n\kappa|r^s|n\kappa \rangle \), \( B^s = \langle n\kappa|\sigma_r r^s|n\kappa \rangle \), and \( C^s = \langle n\kappa|\sigma_t r^s|n\kappa \rangle \) [7–9].

Finally, for the \( ns \) state, we obtain

\[
Q_\mu(ns, Z, I, \mu) = \frac{4m_e \mu}{5Z} \mu_N \left\{ \frac{1}{6(m_e + E_{n,-1})} \left( \frac{4E_{n,-1}^2 + m_e^2}{m_e - E_{n,-1}} \frac{(\alpha Z)^2}{m_e - E_{n,-1}} \right) + \frac{3E_{n,-1}m_e - 2E_{n,-1}^2}{m_e^2} \right\} Q_1
\]

and

\[
Q_Q(ns, Z, I, Q_N) = \frac{5\tau Q_N}{12Z m_e^2 (15 - 16(\alpha Z)^2)(45 + 4(\alpha Z)^2)(m_e^2 - E_{n,-1}^2)}
\]

\[
\times \left\{ 10(-1728E_{n,-1}^4 - 3537m_e E_{n,-1}^3 + 6237E_{n,-1}^2 m_e^2 + 1809E_{n,-1}m_e^3 
- 2457m_e^4) + \frac{3(\alpha Z)^2}{m_e^2 - E_{n,-1}^2} (7405m_e^6 - 736E_{n,-1}^6 + 10528m_e E_{n,-1}^5
- 31033E_{n,-1}^2m_e^4 + 2406E_{n,-1}^3m_e^3 - 3934E_{n,-1}m_e^5 + 20764E_{n,-1}^4m_e^2)
+ \frac{(\alpha Z)^4m_e^2}{m_e^2 - E_{n,-1}^2} (6505m_e^5 - 1120E_{n,-1}^3m_e^2 + 2240E_{n,-1}^4m_e^4 + 1280E_{n,-1}^5
+ 7872m_e E_{n,-1}^4 - 1612E_{n,-1}^2m_e^3) + \frac{400(\alpha Z)^6m_e^4}{m_e^2 - E_{n,-1}^2} (m_e^2 + 4E_{n,-1}^2) \right\}.
\]

It can be seen that formula (11) is a particular case \((n = 1, F = 1, I = 1/2, (\eta = 1))\) of formula (21).

For small \( Z \), we can expand (21) and (22) in the parameter \( \alpha Z \) with the two lowest-order terms kept:

\[
Q_\mu(ns, Z, I, \mu) = \frac{\eta \mu}{3Z} \mu_N \left\{ (n^2 + 2) - (\alpha Z)^2 \left( n - \frac{9}{20} \left( 1 - \frac{1}{n^2} \right) \right) + O((\alpha Z)^4) \right\} Q_1.
\]

\[
Q_Q(ns, Z, I, Q_N) = \tau Q_N \left\{ \frac{61}{36} n^4 - \frac{355}{36} n^2 + 4 
+ \frac{(\alpha Z)^2}{540 n^2} \left( 1028n^6 - 1830n^5 - 4322n^4 + 5325n^3 + 3957n^2 - 2808 \right) + O((\alpha Z)^4) \right\}.
\]
\[ Q_Q(n_{1/2}, Z, I, Q_N) = \frac{5\tau Q_N}{12Z m_e^2(15 - 16(\alpha Z)^2)(45 + 4(\alpha Z)^4)(m_e - E_{n,1})} \]
\[ \times \left\{ 54\left( -76E_{n,1}^3 + 311m_e E_{n,1}^2 + 6m_e^2 E_{n,1} - 141m_e^3 \right) \right. \]
\[ + \left. \frac{3(\alpha Z)^2}{(m_e^2 - E_{n,1}^2)(m_e - E_{n,1})} \right\{ (11805m_e^6 - 41297E_{n,1}m_e^4 - 6112m_eE_{n,1}^5 + 10710E_{n,1}^2m_e^5 - 21132E_{n,1}^4m_e^2 - 998E_{n,1}^3m_e^3 - 640E_{n,1}^6) \right. \]
\[ + \frac{(\alpha Z)^4m_e^2}{(m_e^2 - E_{n,1}^2)(m_e - E_{n,1})} \right\} \left( 7785m_e^4 + 1248m_eE_{n,1}^3 - 288E_{n,1}m_e^3 \right. \]
\[ - 4460E_{n,1}^2m_e^2 + 8000E_{n,1}^4 \right. \left. \right\} \left( \frac{400(\alpha Z)^6m_e^4}{(m_e^2 - E_{n,1}^2)(m_e - E_{n,1})} \right) (m_e^2 + 4E_{n,1}^2) \right\}. \] (26)

For \( n = 2, F = 1, I = 1/2 \) formula (25) agrees with equation (5). For small \( Z \), we can expand expressions (25) and (26) in the parameter \( \alpha Z \) with the two lowest-order terms kept:

\[ Q_\mu(n_{1/2}, Z, I, \mu) = -\frac{\eta \mu}{3Z \mu_N (\alpha Z)^2} \left\{ 4(n^4 - n^2) \right. \]
\[ - (\alpha Z)^2\left( 8n^3 - \frac{19}{3}n^2 - 4n + \frac{4}{5} \right) + O((\alpha Z)^4) \right\} Q_1. \] (27)

\[ Q_Q(n_{1/2}, Z, I, Q_N) = -\frac{\tau Q_N}{(\alpha Z)^2 Z} \left\{ \frac{20}{3} n^2(n^2 - 1) \right. \]
\[ + \frac{(\alpha Z)^2}{12} \left( 65n^4 - 160n^3 - 51n^2 + 80n + 100 \right) + O((\alpha Z)^4) \right\}. \] (28)

### 3 Numerical results

In Tables 1 and 2, we present the numerical results for \( Q_\mu, Q_Q \), and \( Q_{\text{total}} = \frac{2\pi}{2} Q_N + Q_\mu + Q_Q \) (the total quadrupole moment of the atom) for a wide range of hydrogenlike ions. For ions with \( I = 1/2 \), the total quadrupole moment is completely determined by \( Q_{\text{M}_{\mu}} \). For the other ions, the role of the induced quadrupole moment is most important for low \( Z \) and decreases with \( Z \) increasing.

We note also that, according to formulas (25), (27), (24), (28), the induced quadrupole moment increases rapidly with \( n \) increasing. As a result, for highly exited states the total quadrupole moment of a hydrogenlike atom is mainly determined by the induced quadrupole moment.

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Table 1: The numerical results for the $Q_{M\mu}$, the $Q_{MQ}$, and $Q_{\text{total}}$ in case of the 1s state. The values of $\mu/\mu_N$ and $Q_N$ are taken from [10].

| Ion | $^1\text{H}$ | $^{13}\text{C}^{5+}$ | $^{17}\text{O}^{2+}$ | $^{43}\text{Ca}^{19+}$ |
|-----|---------------|-----------------|-----------------|-----------------|
| Z   | 1             | 6               | 8               | 20              |
| I   | 1/2           | 1/2             | 5/2             | 7/2             |
| $\mu/\mu_N$ | 2.79285       | 0.702412(2)    | -1.8938(1)      | -1.3176         |
| $Q_N$, barn | 0             | 0               | -0.02578        | -0.049(5)       |
| $Q_{\mu}$, $F = I + 1/2$, barn | 0.7560         | 0.03167         | -0.06401        | -0.01771        |
| $Q_{Q}$, $F = I + 1/2$, barn | 0             | 0               | 0.001072        | 0.0008(1)       |
| $Q_{\text{total}}$, $F = I + 1/2$, barn | 0.7560         | 0.03167         | -0.08872        | -0.066(5)       |
| $Q_{\mu}$, $F = I - 1/2$, barn | 0             | 0               | 0.02560         | 0.009485        |
| $Q_{Q}$, $F = I - 1/2$, barn | 0             | 0               | 0.0008576       | 0.0007(1)       |
| $Q_{\text{total}}$, $F = I - 1/2$, barn | 0             | 0               | 0.00583         | -0.033(5)       |

| Ion | $^{131}\text{Xe}^{54+}$ | $^{207}\text{Pb}^{81+}$ | $^{209}\text{Bi}^{82+}$ | $^{235}\text{U}^{91+}$ |
|-----|--------------------------|--------------------------|--------------------------|--------------------------|
| Z   | 54                       | 82                       | 83                       | 92                       |
| I   | 3/2                      | 1/2                      | 9/2                      | 7/2                      |
| $\mu/\mu_N$ | 0.691862(4)             | 0.592583(9)             | 4.1106(2)                | -0.39(7)                 |
| $Q_N$, barn | -0.120(12)              | 0                        | -0.50(8)                 | 4.936(6)                 |
| $Q_{\mu}$, $F = I + 1/2$, barn | 0.003281             | 0.001697                 | 0.01158                 | -0.0009(2)               |
| $Q_{Q}$, $F = I + 1/2$, barn | 0.0007(1)             | 0                        | 0.0014(2)               | -0.01095(1)              |
| $Q_{\text{total}}$, $F = I + 1/2$, barn | -0.12(1)              | 0.001697                 | -0.49(8)                | 4.924(6)                 |
| $Q_{\mu}$, $F = I - 1/2$, barn | -0.0005469            | 0                        | -0.007206               | 0.0005(1)                |
| $Q_{Q}$, $F = I - 1/2$, barn | 0.00033(3)            | 0                        | 0.0013(2)               | -0.00978(1)              |
| $Q_{\text{total}}$, $F = I - 1/2$, barn | -0.06(1)              | 0                        | -0.47(7)                | 4.398(5)                 |

1 An average of the values given in [10].
Table 2: The numerical results for the QM$_\mu$, the QM$_Q$, and $Q_{\text{total}}$ in case of the 2p$_{1/2}$ state. The values of $\mu/\mu_N$ and $Q_N$ are taken from [10].

| Ion          | $^1$H | $^{13}$C$^{5+}$ | $^{17}$O$^{5+}$ | $^{43}$Ca$^{19+}$ |
|--------------|------|----------------|----------------|-----------------|
| $Z$          | 1    | 6              | 8              | 20              |
| $I$          | 1/2  | 1/2            | 5/2            | 7/2             |
| $\mu/\mu_N$ | 2.79285 | 0.702412(2) | -1.8938(1) | -1.3176         |
| $Q_N$, barn  | 0    | 0              | -0.02578       | -0.049(5)       |
| $Q_{\mu}, F = I + 1/2$, barn | -227170(100) | -264.1 | 300.0 | 13.15 |
| $Q_Q, F = I + 1/2$, barn | 0 | 0 | 6.051 | 0.73(8) |
| $Q_{\text{total}, F = I + 1/2}$, barn | -227170(100) | -264.1 | 306.0 | 13.83(8) |
| $Q_{\mu}, F = I - 1/2$, barn | 0 | 0 | -120.0 | -7.044 |
| $Q_Q, F = I - 1/2$, barn | 0 | 0 | 4.838 | 0.65(8) |
| $Q_{\text{total}, F = I - 1/2}$, barn | 0 | 0 | -115.2 | -6.44(8) |

| Ion          | $^{131}$Xe$^{54+}$ | $^{207}$Pb$^{84+}$ | $^{209}$Bi$^{82+}$ | $^{235}$U$^{91+}$ |
|--------------|--------------------|--------------------|--------------------|--------------------|
| $Z$          | 54                 | 82                 | 83                 | 92                 |
| $I$          | 3/2                | 1/2                | 9/2                | 7/2                |
| $\mu/\mu_N$ | 0.691862(4)        | 0.592583(9)        | 4.1106(2)          | -0.39(7)           |
| $Q_N$, barn  | -0.120(12)         | 0                  | -0.50(8)           | 4.936(6)           |
| $Q_{\mu}, F = I + 1/2$, barn | -0.3096 | -0.06061 | -0.4015 | 0.025(5) |
| $Q_Q, F = I + 1/2$, barn | 0.09(1) | 0 | 0.10(3) | -0.723(1) |
| $Q_{\text{total}, F = I + 1/2}$, barn | -0.34(1) | -0.06061 | -0.8(1) | 4.24(1) |
| $Q_{\mu}, F = I - 1/2$, barn | 0.05160 | 0 | 0.2598 | -0.013(5) |
| $Q_Q, F = I - 1/2$, barn | 0.045(5) | 0 | 0.093(15) | -0.645(1) |
| $Q_{\text{total}, F = I - 1/2}$, barn | 0.04(1) | 0 | -0.11(9) | 3.75(1) |

1 An average of the values given in [10].