Magnetic field-induced electric quadrupole moment in the ground state of the relativistic hydrogen-like atom: Application of the Sturmian expansion of the generalized Dirac–Coulomb Green function

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Abstract

We consider a Dirac one-electron atom placed in a weak, static, uniform magnetic field. We show that, to the first order in the strength $B$ of the perturbing field, the only electric multipole moment induced by the field in the ground state of the atom is the quadrupole one. Using the Sturmian expansion of the generalized Dirac–Coulomb Green function [R. Szmytkowski, J. Phys. B 30 (1997) 825; erratum 30 (1997) 2747], we derive a closed-form expression for the induced electric quadrupole moment. The result contains the generalized hypergeometric function $_3F_2$ of the unit argument. Earlier calculations by other authors, based on the non-relativistic model of the atom, predicted in the low-field region the quadratic dependence of the induced electric quadrupole moment on $B$.

Key words: electric quadrupole moment; magnetic field; Zeeman effect; Dirac one-electron atom; Dirac–Coulomb Green function; Sturmian functions

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1 Introduction

In the mid 1950’s, Coulson and Stephen [1] pointed out that the uniform magnetic field should induce the electric quadrupole moment (EQM) in the hydrogen-like atom. They used the perturbation theory and found that in the case of the non-relativistic atom, for field strengths $B$ corresponding to the complete Paschen–Back effect, the leading term in the expansion of the induced EQM in powers of the field strength is quadratic in $B$. For the atomic ground state, their result, after being translated into the form conforming both to the definition of the EQM (cf. Sec. 3 below) and to the notation used in the present work, is

$$Q_{20} \simeq Q^{(2)}_{20} = -\frac{5}{16} \frac{\alpha^4 e a_0^3 B^2}{Z^6 B_0^2},$$

where $Ze$ is the nuclear charge, $a_0$ is the Bohr radius, $\alpha$ is the Sommerfeld fine-structure constant, whereas

$$B_0 = \frac{\mu_0 \mu_B}{4\pi a_0^3} = \frac{\alpha^2 \hbar}{2 e a_0^2} \simeq 6.26 \text{ T}$$

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is the atomic unit of the magnetic induction ($\mu_0$ is the vacuum permeability and $\mu_B$ is the Bohr magneton). Later, Turbiner [2, Sec. 5] arrived at the same expression for $Q_{20}^{(2)}$ for the Schrödinger one-electron atom with $Z = 1$ and found also explicitly the next non-vanishing term (being $Q_{20}^{(4)} \sim B^4$) in the expansion of $Q_{20}$ in powers of $B$. Moreover, using the variational technique, he determined the function $Q_{20}(B)$ for magnetic fields ranging from vanishing to superstrong. A decade ago, Potekhin and Turbiner [3] calculated $Q_{20}(B)$, over a still broader range of $B$, by two different methods, one being the variational approach with a more sophisticated trial function than the one used in Ref. [2], the other being based on the expansion of the perturbed electronic wave function in the Landau orbitals. In the low-field limit, the results of Ref. [3] reproduced the quadratic dependence of the induced EQM on $B$ predicted in Refs. [1, 2].

In all the aforementioned works, the atom has been described non-relativistically. In the present paper, we show that if the relativity is taken into account and the atomic model adopted is the one based on the Dirac equation for the electron, it appears that the weak, static, uniform magnetic field induces in the ground state of the atom the EQM which, to the lowest order, is linear in the perturbing field strength $B$; no other electric multipole moments are induced in the system to the first order in $B$. Exploiting the Sturmian expansion of the generalized (or reduced) Dirac–Coulomb Green function, found by one of us in Ref. [4] and subsequently successfully used in analytical calculations of various electromagnetic properties of the Dirac one-electron atom [5–9], in Sec. 4 we derive a closed-form expression for the induced EQM, in terms of the generalized hypergeometric function $\,_{3}F_{2}$ with the unit argument.

## 2 Preliminaries

It has been already stated in the introduction that the system we shall be concerned with in the present work is the Dirac one-electron atom. Its nucleus will be assumed to be point-like, infinitely heavy, spinless, and to carry the electric charge $Ze$. In the absence of external perturbations, the atomic ground-state energy level

$$E^{(0)} = mc^2 \gamma_1,$$

where

$$\gamma_\kappa = \sqrt{\kappa^2 - (\alpha Z)^2},$$

is two-fold degenerate, the two associated Hamiltonian eigenfunctions, orthonormal in the sense of

$$\int \mathbb{R}^3 d^3r \, \Psi^{(0)\dagger}_\mu(r) \Psi^{(0)}_{\mu'}(r) = \delta_{\mu\mu'},$$

being

$$\Psi^{(0)}_\mu(r) = \frac{1}{r} \left( \begin{array}{c} P^{(0)}(r) \Omega_{-1\mu}(n_r) \\ iQ^{(0)}(r) \Omega_{1\mu}(n_r) \end{array} \right) \quad (\mu = \pm \frac{1}{2}).$$

The radial functions appearing in Eq. (2.4), normalized according to

$$\int_0^\infty dr \left\{ [P^{(0)}(r)]^2 + [Q^{(0)}(r)]^2 \right\} = 1,$$

are explicitly given by

$$P^{(0)}(r) = -\sqrt{\frac{Z}{a_0 \Gamma(2\gamma_1 + 1)}} \left( \frac{2Zr}{a_0} \right)^{\gamma_1} e^{-Zr/a_0},$$

$$Q^{(0)}(r) = \sqrt{\frac{Z}{a_0 \Gamma(2\gamma_1 + 1)}} \left( \frac{2Zr}{a_0} \right)^{\gamma_1} e^{-Zr/a_0},$$

whereas $\Omega_{\kappa\mu}(n_r)$, with $n_r = r / r$, are the orthonormal spherical spinors defined as in Ref. [10].
In the presence of a weak, static, uniform magnetic field $B = Bn_z$, the level $E^{(0)}$ splits into two. Their energies, to the first order in $B$, are given by

$$E_\mu \simeq E^{(0)} + E^{(1)}_\mu \quad (\mu = \pm \frac{1}{2}),$$

with

$$E^{(1)}_\mu = \operatorname{sgn}(\mu) \frac{2\gamma_1 + 1}{3} \mu_B B. \quad (2.8)$$

The corresponding wave functions, to the same approximation order, are

$$\Psi_\mu(r) \simeq \Psi^{(0)}_\mu(r) + \Psi^{(1)}_\mu(r) \quad (\mu = \pm \frac{1}{2}).$$

Here, the zeroth-order component $\Psi^{(0)}_\mu(r)$ is given by Eq. (2.4) (the space quantization axis is now chosen to be directed along $B$). The correction $\Psi^{(1)}_\mu(r)$ solves the inhomogeneous differential equation

$$\left[-i\hbar \alpha \cdot \nabla + \beta mc^2 - \frac{Ze^2}{(4\pi \epsilon_0)^{1/2}} - E^{(0)}\right] \Psi^{(1)}_\mu(r) = - \frac{1}{2} e c \alpha \cdot (B \times r) - E^{(1)}_\mu \Psi^{(0)}_\mu(r) \quad (2.10)$$

($\alpha$ and $\beta$ are the standard Dirac matrices), subject to the usual regularity conditions and the orthogonality constraint

$$\int_{\mathbb{R}^3} d^3r \Psi^{(0)*}_\mu(r) \Psi^{(1)}_{\mu'}(r) = 0 \quad (\mu, \mu' = \pm \frac{1}{2}). \quad (2.11)$$

The integral representation of $\Psi^{(1)}_\mu(r)$ is

$$\Psi^{(1)}_\mu(r) = -\frac{1}{2} e c B \cdot \int_{\mathbb{R}^3} d^3r' G^{(0)}(r, r') (r' \times \alpha) \Psi^{(0)}_{\mu'}(r'),$$

where $G^{(0)}(r, r')$ is the generalized Dirac–Coulomb Green function associated with the ground-state energy level (2.1).

### 3 Analysis of electric multipole moments of the atom in the magnetic field

After these preparatory steps, we set the problem: which electric multipole moments, apart from the monopole one, characterize the electronic cloud of the atom in the perturbed state $\Psi_\mu(r)$? If $\rho_\mu(r)$ is the electronic charge density for that state, the spherical components of the $L$-th order electric multipole moment tensor are defined as

$$Q_{LM\mu} = \sqrt{\frac{4\pi}{2L + 1}} \int_{\mathbb{R}^3} d^3r r^L Y^*_L M(n_r) \rho_\mu(r), \quad (3.1)$$

where the asterisk denotes the complex conjugation and $Y^*_L M(n_r)$ is the normalized spherical harmonic defined according to the Condon–Shortley phase convention [11, chapter 5]. For the atom being in the state $\Psi_\mu(r)$, the density $\rho_\mu(r)$ is given by

$$\rho_\mu(r) = \frac{-e \Psi^{(0)*}_\mu(r) \Psi_\mu(r)}{\int_{\mathbb{R}^3} d^3r' \Psi^{(0)*}_{\mu'}(r') \Psi_{\mu'}(r')} \quad (3.2)$$

Using Eqs. (2.9) and (2.11), to the first order in the perturbing field, one has

$$\rho_\mu(r) \simeq \rho^{(0)}_\mu(r) + \rho^{(1)}_\mu(r), \quad (3.3)$$

with

$$\rho^{(0)}_\mu(r) = -e \Psi^{(0)*}_\mu(r) \Psi^{(0)}_\mu(r) \quad (3.4)$$
and
\[ \rho_{\mu}^{(1)}(r) = -e \left[ \Psi_{\mu}^{(1)}(r) \Psi_{\mu}^{(0)}(r) + \Psi_{\mu}^{(0)}(r) \Psi_{\mu}^{(1)}(r) \right]. \]  

(3.5)

Accordingly, it follows that
\[ Q_{LM\mu} \simeq Q_{LM\mu}^{(0)} + Q_{LM\mu}^{(1)}, \]
\[ Q_{LM\mu}^{(0)} = -e \sqrt{\frac{4\pi}{2L+1}} \int_{\mathbb{R}^3} d^3r \Psi_{\mu}^{(0)}(r) r^L Y_{LM}(n_r) \Psi_{\mu}^{(0)}(r). \]
\[ (3.7) \]

is the multipole moment for the unperturbed atom, whereas
\[ Q_{LM\mu}^{(1)} = Q_{LM\mu}^{(1)} + (-)^M Q_{LM-M\mu}^{(1)}, \]
\[ (3.8) \]

with
\[ Q_{LM\mu}^{(1)} = -e \sqrt{\frac{4\pi}{2L+1}} \int_{\mathbb{R}^3} d^3r \Psi_{\mu}^{(0)}(r) r^L Y_{LM}(n_r) \Psi_{\mu}^{(1)}(r), \]
\[ (3.9) \]

is the first-order correction induced by the perturbing magnetic field. To arrive at Eq. (3.8), we have exploited the well-known identity
\[ Y_{LM}(n_r) = (-)^M Y_{LM-M}(n_r). \]
\[ (3.10) \]

If the representation (2.12) of \( \Psi_{\mu}^{(1)}(r) \) is plugged into Eq. (3.9), this gives \( Q_{LM\mu}^{(1)} \) in the form of the double integral over \( \mathbb{R}^3 \):
\[ Q_{LM\mu}^{(1)} = \frac{1}{2} \sqrt{\frac{4\pi}{2L+1}} e^2 \epsilon B \int_{\mathbb{R}^3} d^3r \int_{\mathbb{R}^3} d^3r' \Psi_{\mu}^{(0)}(r) r^L Y_{LM}(n_r) \Psi_{\mu}^{(1)}(r'), \]
\[ (3.11) \]

Using Eq. (2.4) and the explicit representations of the spherical spinors \( \Omega_{\pm 1\mu}(n_r) \), it is easy to show that the electronic charge density in the unperturbed atom, \( \rho_{\mu}^{(0)}(r) \), is spherically symmetric and the integral in Eq. (3.7) differs from zero only if \( L = 0 \) and \( M = 0 \). Hence, for the ground state of the unperturbed atom it holds that
\[ Q_{LM\mu}^{(0)} = -e \delta_{LM} \delta_{M0}, \]
\[ (3.12) \]

i.e., all permanent electric multipole moments of the electronic cloud other than the monopole one do vanish.

Next, we proceed to the analysis of the first-order induced multipole moments \( Q_{LM\mu}^{(1)} \). To this end, we have to invoke the multipole representation of the generalized Green function, which is
\[ \bar{G}^{(0)}(r, r') = \frac{4\pi \epsilon_0}{e^2} \sum_{|\kappa|=-\infty}^{r} \sum_{m=|\kappa|+1/2}^{r} \frac{1}{r r'} \times \left( \begin{array}{cc} g^{(0)}_{\kappa(+\kappa)}(r, r') \Omega_{\kappa\mu}(n_r) \Omega_{\kappa\mu}^{\dagger}(n_r') & -i g^{(0)}_{\kappa(+\kappa)}(r, r') \Omega_{\kappa\mu}(n_r) \Omega_{\kappa\mu}^{\dagger}(n_r') \\ i g^{(0)}_{\kappa(-\kappa)}(r, r') \Omega_{-\kappa\mu}(n_r) \Omega_{-\kappa\mu}^{\dagger}(n_r') & g^{(0)}_{\kappa(-\kappa)}(r, r') \Omega_{-\kappa\mu}(n_r) \Omega_{-\kappa\mu}^{\dagger}(n_r') \end{array} \right). \]
\[ (3.13) \]

If Eqs. (2.4) and (3.13) are inserted into Eq. (3.11), the angular integration in the resulting formula may be conveniently carried out with the aid of the identity [10, Eq. (3.1.6)]
\[ n_z \cdot (n_r \times \sigma) \Omega_{\kappa\mu}(n_r) = i \frac{4\mu \kappa}{4\kappa^2 - 1} \Omega_{\kappa\mu}(n_r) + i \frac{\sqrt{(\kappa + \frac{1}{2})^2 - \mu^2}}{|2\kappa + 1|} \Omega_{\kappa+1\mu}(n_r) \\
- i \frac{\sqrt{(\kappa - \frac{1}{2})^2 - \mu^2}}{|2\kappa - 1|} \Omega_{\kappa-1\mu}(n_r) \]
\[ (3.14) \]
and the relation
\[
\sqrt{\frac{4\pi}{2L+1}} \int \frac{d^2r}{4\pi} \, d^3r \, \Omega_{\mu}^\dagger(n_r) Y_{LM}(n_r) \Omega_{\mu'}(n_r) \\
= (-)^{\mu'+1/2} \sqrt{|\kappa\kappa'|} \left( \begin{array}{ccc} |\kappa| - \frac{1}{2} & L & |\kappa'| - \frac{1}{2} \\ -\frac{1}{2} & 0 & \frac{1}{2} \end{array} \right) \left( \begin{array}{ccc} |\mu| - \frac{1}{2} & M & |\mu'| - \frac{1}{2} \\ -\mu' \end{array} \right) \Pi(l, L', l'),
\]
(3.15)
with
\[
\Pi(l, L, l') = \left\{ \begin{array}{ll} 1 & \text{for } l + L + l' \text{ even} \\ 0 & \text{for } l + L + l' \text{ odd}. \end{array} \right.
\]
(3.16)
In Eq. (3.15), \( \left( \begin{array}{ccc} j_a & j_b & j_c \\ m_a & m_b & m_c \end{array} \right) \) denotes the Wigner’s 3j coefficient, whereas
\[
l = \left| \kappa + \frac{1}{2} \right| - \frac{1}{2},
\]
(3.17)
and similarly for \( l' \). Exploiting the selection rules embodied in Eq. (3.16) and properties of the 3j coefficients, one deduces that the only case when \( \widetilde{Q}_{LM\mu}^{(1)} \) does not vanish is the one with \( L = 2 \) and \( M = 0 \). Since \( \widetilde{Q}_{20\mu}^{(1)} \) is real, from Eq. (3.8) one has
\[
\widetilde{Q}_{LM\mu}^{(1)} = \widetilde{Q}_{20\mu}^{(1)} \delta_{L2} \delta_{M0},
\]
(3.18)
with \( \widetilde{Q}_{20\mu}^{(1)} \) being given in the form of the following double radial integral:
\[
\widetilde{Q}_{20\mu}^{(1)} = \text{sgn}(\mu) \frac{2}{15} (4\pi\epsilon_0)cB \int_0^\infty dr \int_0^\infty dr' \left( \begin{array}{cc} P^{(0)}(r) & Q^{(0)}(r) \end{array} \right) r^2 \bar{G}_{20}^{(0)}(r, r') \left( \begin{array}{cc} Q^{(0)}(r') \\ P^{(0)}(r') \end{array} \right),
\]
(3.19)
where
\[
\bar{G}_{20}^{(0)}(r, r') = \left( \begin{array}{cc} \bar{g}_{20}^{(0)}(r, r') & \bar{g}_{20}^{(0)}(r, r') \\ \bar{g}_{20}^{(0)}(r, r') & \bar{g}_{20}^{(0)}(r, r') \end{array} \right)
\]
(3.20)
is the radial generalized Green function.

4 Evaluation of the induced electric quadrupole moment

In the preceding section, we have proved that, to the first order in \( B \), the only electric multipole moment induced in the electronic cloud of the atom by the weak, static, uniform magnetic field is the quadrupole \( (L = 2) \) one, and that its only non-vanishing spherical component is the one with \( M = 0 \). Now, the Cartesian components of the traceless tensor of the induced quadrupole moment, \( Q_{ij}^{(1)} \)
\[
Q_{ij}^{(1)} = \int_{\mathbb{R}^3} d^3r \frac{1}{2} (3r_i r_j - r^2 \delta_{ij}) \rho_{\mu}^{(1)}(r) \quad (i, j \in \{x, y, z\}),
\]
(4.1)
are related to its spherical components through
\[
\left( \begin{array}{cccc} Q_{x2\mu}^{(1)} & Q_{y2\mu}^{(1)} & Q_{z2\mu}^{(1)} \\ Q_{2x\mu}^{(1)} & Q_{y2\mu}^{(1)} & Q_{z2\mu}^{(1)} \\ Q_{2y\mu}^{(1)} & Q_{2y\mu}^{(1)} & Q_{2z\mu}^{(1)} \end{array} \right) = \left( \begin{array}{ccc} -\frac{1}{2} Q_{20\mu}^{(1)} + \sqrt{\frac{7}{8}} [Q_{22\mu}^{(1)} + Q_{2-2\mu}^{(1)}] & i \sqrt{\frac{3}{8}} [Q_{22\mu}^{(1)} - Q_{2-2\mu}^{(1)}] & -i \sqrt{\frac{3}{8}} [Q_{21\mu}^{(1)} - Q_{2-1\mu}^{(1)}] \\ i \sqrt{\frac{3}{8}} [Q_{22\mu}^{(1)} - Q_{2-2\mu}^{(1)}] & -\frac{1}{2} Q_{20\mu}^{(1)} - \sqrt{\frac{3}{8}} [Q_{22\mu}^{(1)} + Q_{2-2\mu}^{(1)}] & -i \sqrt{\frac{3}{8}} [Q_{21\mu}^{(1)} + Q_{2-1\mu}^{(1)}] \\ -i \sqrt{\frac{3}{8}} [Q_{21\mu}^{(1)} - Q_{2-1\mu}^{(1)}] & -i \sqrt{\frac{3}{8}} [Q_{21\mu}^{(1)} + Q_{2-1\mu}^{(1)}] & \frac{1}{2} Q_{20\mu}^{(1)} \end{array} \right).
\]
(4.2)
Hence, it follows that in the Cartesian basis all the off-diagonal elements of the quadrupole moment induced in the system under study do vanish:

\[
Q_{ij\mu}^{(1)} = 0 \quad (i \neq j; i, j \in \{x, y, z\}),
\]

while the diagonal elements are given by

\[
Q_{xx\mu}^{(1)} = Q_{yy\mu}^{(1)} = -\frac{1}{2} Q_{zz\mu}^{(1)} = -\frac{1}{2} Q_{20\mu}^{(1)}.
\]

Such a structure of the Cartesian representation of the quadrupole moment tensor is characteristic for systems possessing the rotational symmetry around the z axis (recall that in our case the z axis is directed along the magnetic field).

It remains to evaluate the double integral in Eq. (3.19). For this purpose, we shall make use of the Sturmian expansion of the pertinent generalized radial Dirac–Coulomb Green function for the atomic ground state, which is [4]

\[
\mathcal{G}_{\kappa}^{(0)} (r, r') = \sum_{n_r=0}^{\infty} \frac{1}{\mu_{n_r, \kappa} - 1} \left( \frac{S_{\kappa, n_r}^{(0)} (r)}{T_{\kappa, n_r}^{(0)} (r)} \right) \left( \mu_{n_r, \kappa} S_{\kappa, n_r}^{(0)} (r') T_{\kappa, n_r}^{(0)} (r') \right) \quad (\kappa \neq -1).
\]

Here

\[
S_{\kappa, n_r}^{(0)} (r) = \sqrt{\frac{(1 + \gamma_1)(|n_r| + 2\gamma_2)|n_r|!}{2Z N_{n_r, \kappa} (N_{n_r, \kappa} - \kappa) \Gamma(|n_r| + 2\gamma_2)}} \times \left( \frac{2Zr}{a_0} \right)^{\gamma_2 - \gamma_1} e^{-Zr/a_0} \left[ L_{|n_r| - 1}^{(2\gamma_2)} \left( \frac{2Zr}{a_0} \right) + \frac{\kappa - N_{n_r, \kappa} f_{|n_r|}^{(2\gamma_2)}}{|n_r| + 2\gamma_2} \right] \right]
\]

and

\[
T_{\kappa, n_r}^{(0)} (r) = \sqrt{\frac{(1 - \gamma_1)(|n_r| + 2\gamma_2)|n_r|!}{2Z N_{n_r, \kappa} (N_{n_r, \kappa} - \kappa) \Gamma(|n_r| + 2\gamma_2)}} \times \left( \frac{2Zr}{a_0} \right)^{\gamma_2 - \gamma_1} e^{-Zr/a_0} \left[ L_{|n_r| - 1}^{(2\gamma_2)} \left( \frac{2Zr}{a_0} \right) - \frac{\kappa - N_{n_r, \kappa} f_{|n_r|}^{(2\gamma_2)}}{|n_r| + 2\gamma_2} \right] \right)
\]

[with \( L^{(\alpha)}_{\kappa} (x) \) denoting the generalized Laguerre polynomial [12]; we define \( L^{(\alpha)}_{-1} (\rho) \equiv 0 \)] are the radial Dirac–Coulomb Sturmian functions associated with the hydrogenic ground-state energy level, whereas

\[
\mu_{n_r, \kappa} = \frac{|n_r| + \gamma_2 + N_{n_r, \kappa}}{\gamma_1 + 1},
\]

with

\[
N_{n_r, \kappa} = \pm \sqrt{(|n_r| + \gamma_2)^2 + (\alpha Z)^2} = \pm \sqrt{|n_r|^2 + 2|n_r| \gamma_2 + \kappa^2}
\]

being the ‘apparent principal quantum number’ (notice that it may assume positive as well as negative values!); the following sign convention applies to the definition (4.8): the plus sign should be chosen for \( n_r > 0 \) and the minus one for \( n_r < 0 \); for \( n_r = 0 \) one chooses the plus sign if \( \kappa < 0 \) and the minus sign if \( \kappa > 0 \). Insertion of the separable expansion (4.5) into the right-hand side of the formula in Eq. (3.19) leads to the following expression for \( Q_{20\mu}^{(1)} \):

\[
Q_{20\mu}^{(1)} = \text{sgn}(\mu) \frac{2}{15} (4\pi e_0) e B \sum_{n_r=-\infty}^{\infty} \frac{1}{\mu_{n_r, 2}^{(0)} - 1} \int_0^{\infty} dr \int_0^{\infty} dr' \left[ P^{(0)}(r) S_{n_r, 2}^{(0)} (r) + Q^{(0)}(r) T_{n_r, 2}^{(0)} (r) \right] \times \mu_{n_r, 2}^{(0)} Q^{(0)}(r') S_{n_r, 2}^{(0)} (r') + P^{(0)}(r') T_{n_r, 2}^{(0)} (r') \right].
\]

The radial integrals in Eq. (4.9) may be taken after one makes use of Eq. (4.7) and of the explicit representations of the radial functions \( P^{(0)}(r) \), \( Q^{(0)}(r) \) and the radial Sturmians \( S_{n_r, 2}^{(0)} (r) \),
and the trivial but extremely useful identity
\[ \gamma_2^2 = \gamma_1^2 + 3, \]  
(4.11)

one arrives at
\[
Q_{20\mu}^{(1)} = -\text{sgn}(\mu) \frac{\alpha^2 e a_0^2}{Z^4} \frac{B}{B_0} \frac{\Gamma^2(\gamma_1 + \gamma_2 + 3)}{480(4\gamma_1 + 1)\Gamma(2\gamma_1 + 1)\Gamma^2(\gamma_2 - \gamma_1 - 2)} \times \left( \sum_{n_r = -\infty}^{\infty} \frac{\Gamma(|n_r| + \gamma_2 - \gamma_1 - 3)\Gamma(|n_r| + \gamma_2 - \gamma_1 - 2)}{|n_r|\Gamma(|n_r| + 2\gamma_2 + 1) N_{n_2}} \times \frac{(|n_r| + \gamma_2 - 3\gamma_1 - 3 - \gamma_1 N_{n_2})(3|n_r| + \gamma_1 + 3\gamma_2 + 1 + 3N_{n_2})}{|n_r| + \gamma_2 - \gamma_1 - 1 + N_{n_2}} \right). 
\]
(4.12)

The above result may be simplified considerably if in the series \(\sum_{n_r = -\infty}^{\infty} \cdots\) one collects together terms with the same absolute value of the summation index \(n_r\) (the Sturmian radial quantum number). Proceeding in that way, after much labor, using Eq. (4.8) and again the identity (4.11), one finds that
\[
Q_{20\mu}^{(1)} = -\text{sgn}(\mu) \frac{\alpha^2 e a_0^2}{Z^4} \frac{B}{B_0} \frac{\Gamma^2(\gamma_1 + \gamma_2 + 3)}{240(4\gamma_1 + 1)\Gamma(2\gamma_1 + 1)\Gamma^2(\gamma_2 - \gamma_1 - 2)} \times \left( \sum_{n_r = 0}^{\infty} \frac{\Gamma(n_r + \gamma_2 - \gamma_1 - 3)\Gamma(n_r + \gamma_2 - \gamma_1 - 2)}{n_r(\gamma_2 - \gamma_1)\Gamma(n_r + 2\gamma_2 + 1)} \times (2\gamma_1 - 1)(n_r + \gamma_2 - \gamma_1 - 3)(n_r + \gamma_2 - \gamma_1) + 2(\gamma_1 + 1)(2\gamma_1 + 1)(n_r + \gamma_2 - \gamma_1)
\]
\[
- 6(\gamma_1 + 1)).
\]
(4.13)

It is possible to achieve a further simplification. To this end, we express the right-hand side of Eq. (4.13) in terms of the hypergeometric functions \(_2F_1\) and \(_3F_2\) of the unit argument. Since it holds that
\[
\sum_{n = 0}^{\infty} \frac{\Gamma(n + a_1)\Gamma(n + a_2)}{n!(n + b)} = \frac{\Gamma(a_1)\Gamma(a_2)}{\Gamma(b)} \ _2F_1 \left( \begin{array}{c} a_1, a_2 \\ b \end{array} ; 1 \right),
\]
(4.14)

and
\[
\sum_{n = 0}^{\infty} \frac{\Gamma(n + a_1)\Gamma(n + a_2)}{n!(n + a_3)\Gamma(n + b)} = \frac{\Gamma(a_1)\Gamma(a_2)\Gamma(a_3)}{\Gamma(b)} \ _3F_2 \left( \begin{array}{c} a_1, a_2, a_3 \\ a_3 + 1, b \end{array} ; 1 \right),
\]
(4.15)

Eq. (4.13) becomes
\[
Q_{20\mu}^{(1)} = -\text{sgn}(\mu) \frac{\alpha^2 e a_0^2}{Z^4} \frac{B}{B_0} \frac{\Gamma(\gamma_1 + \gamma_2 + 3)\Gamma(\gamma_1 + \gamma_2 + 4)}{1440(4\gamma_1 + 1)(8\gamma_1 + 1)\Gamma(2\gamma_1 + 1)\Gamma(2\gamma_2 + 1)} \times \left[ (2\gamma_1 - 1)(\gamma_2 - \gamma_1 - 3) \ _2F_1 \left( \begin{array}{c} \gamma_2 - \gamma_1 - 2, \gamma_2 - \gamma_1 - 2 \\ 2\gamma_2 + 1 \end{array} ; 1 \right) 
\]
\[
+ 2(\gamma_1 + 1)(2\gamma_1 + 1) \ _2F_1 \left( \begin{array}{c} \gamma_2 - \gamma_1 - 3, \gamma_2 - \gamma_1 - 2 \\ 2\gamma_2 + 1 \end{array} ; 1 \right) 
\]
\[
- \frac{6(\gamma_1 + 1)}{\gamma_2 - \gamma_1} \ _3F_2 \left( \begin{array}{c} \gamma_2 - \gamma_1 - 3, \gamma_2 - \gamma_1 - 2, \gamma_2 - \gamma_1 \\ \gamma_2 - \gamma_1 + 1, 2\gamma_2 + 1 \end{array} ; 1 \right) \right].
\]
(4.16)

The two \(_2F_1\) functions may be then eliminated with the aid of the Gauss’ identity [13, Eq. (9.122.1)]
\[
\ _2F_1 \left( \begin{array}{c} a_1, a_2 \\ b \end{array} ; 1 \right) = \frac{\Gamma(b)\Gamma(b - a_1 - a_2)}{\Gamma(b - a_1)\Gamma(b - a_2)} \text{ [Re}(b - a_1 - a_2) > 0].
\]
(4.17)
After some simple algebra, we obtain

\[
Q_{20\mu}^{(1)} = \text{sgn}(\mu) \frac{2a e_a^2 B}{Z^4 B_0} \frac{\Gamma(2_1 + 5)}{240 \Gamma(2_1 + 1) \Gamma(2_1 + 3)} \left[ -2(2_1^2 + 3_1 + 4) \right.
\]
\[
+ \frac{\Gamma(2_1 + 2) \Gamma(2_1 + 3) \Gamma(2_1 + 4)}{\Gamma(2_1 + 5) \Gamma(2_1 + 7)} \times \gamma_2 - \gamma_1 - 3, \gamma_2 - \gamma_1 - 2, \gamma_2 - \gamma_1 - 1, \gamma_2 + 1 \right] \]
\[
\times \frac{a_1 + 1, a_2, a_3}{a_1 - a_3} \frac{\Gamma(b - a_1 - a_2)}{\Gamma(b - a_1) \Gamma(b - a_2)} - \frac{a_1}{a_1 - a_3} \times \frac{a_{1 + 1}, a_2, a_3}{a_{3 + 1}, b} \right]
\]
\[
\frac{\Gamma(2_1 + 5)}{\Gamma(2_1 + 7)} \times \gamma_2 - \gamma_1 - 2, \gamma_2 - \gamma_1 - 1, \gamma_2 - \gamma_1 - 1, \gamma_2 + 1 \right]
\].

Various other equivalent representations of \(Q_{20\mu}^{(1)}\) may be derived from Eq. (4.18) with the help of recurrence relations obeyed by the \(3F_2(1)\) function. For instance, if one uses repeatedly the relation

\[
3F_2 \left( \begin{array}{c} a_1, a_2, a_3 \\ a_3 + 1, b \end{array}; 1 \right) = \frac{a_3}{a_1 - a_3} \Gamma(b - a_1 - a_2) - \frac{a_1}{a_1 - a_3} \times \frac{a_{1 + 1}, a_2, a_3}{a_{3 + 1}, b} \right]
\]
\[
\frac{\Gamma(b - a_1 - a_2)}{\Gamma(b - a_1) \Gamma(b - a_2)} - \frac{a_1}{a_1 - a_3} \times \frac{a_{1 + 1}, a_2, a_3}{a_{3 + 1}, b} \right]
\]
\[
\frac{\Gamma(2_1 + 5)}{\Gamma(2_2 + 7)} \times \gamma_2 - \gamma_1 - 2, \gamma_2 - \gamma_1 - 1, \gamma_2 - \gamma_1 - 1, \gamma_2 + 1 \right]
\].

Before concluding, it seems worthwhile to investigate the approximation to Eq. (4.20) for \(\alpha Z \ll 1\). Then one has

\[
\gamma_\kappa \simeq |\kappa| - \frac{(\alpha Z)^2}{2|\kappa|} \quad (\kappa \in \mathbb{Z} \setminus \{0\}),
\]

and consequently

\[
\Gamma(\gamma_\kappa + \gamma_\kappa' + k) \simeq \left( |\kappa| + |\kappa'| + k - 1 \right)! \left[ 1 - \frac{1}{2} \left( \frac{1}{|\kappa|} + \frac{1}{|\kappa'|} \right) \psi (|\kappa| + |\kappa'| + k) (\alpha Z)^2 \right]
\]
\[
(\kappa, \kappa' \in \mathbb{Z} \setminus \{0\}, k \in \mathbb{N}),
\]

where

\[
\psi(\zeta) = \frac{1}{\Gamma(\zeta)} \frac{d\Gamma(\zeta)}{d\zeta}
\]

is the digamma function. Using Eq. (4.22) and the recurrence relation

\[
\psi(\zeta + 1) = \psi(\zeta) + \frac{1}{\zeta}
\]

yields

\[
\frac{(\gamma_1 + 1)(\gamma_1 + \gamma_2)\Gamma(\gamma_1 + \gamma_2 + 2)\Gamma(\gamma_1 + \gamma_2 + 3)}{\gamma_1 \Gamma(2_1 + 5) \Gamma(2_1 + 7)} \simeq 1 + \frac{13}{60} (\alpha Z)^2.
\]

Since at the same time, to the second order in \(\alpha Z\), it holds that

\[
3F_2 \left( \begin{array}{c} \gamma_2 - \gamma_1 - 2, \gamma_2 - \gamma_1 - 1, \gamma_2 - \gamma_1 - 1, \gamma_2 + 1 \\ \gamma_2 - \gamma_1 + 1, 2_2 + 1 \end{array}; 1 \right) \simeq 1 - \frac{(\alpha Z)^2}{40},
\]

the sought approximation to \(Q_{20\mu}^{(1)}\) is

\[
Q_{20\mu}^{(1)} \simeq \text{sgn}(\mu) \frac{23 a e_a^2 B}{240 Z^2 B_0} \quad (\alpha Z \ll 1).
\]

It is seen from Eqs. (4.27) and (1.1) that for the hydrogen atom \((Z = 1)\) and for the perturbing magnetic field comparable with the intra-atomic magnetic field, i.e., for \(B \simeq B_0\), the first-order quadrupole moment \(Q_{20\mu}^{(1)}\) predicted by the relativistic formalism is of the same order of magnitude as the second-order moment \(Q_{20\mu}^{(2)}\) obtained from the non-relativistic theory.
5 Conclusions

Earlier calculations of the magnetic field-induced electric quadrupole moment in the ground state of the hydrogen-like atom, based on the non-relativistic atomic model, predicted the quadratic dependence of that moment on the field strength in the low-field regime. In the present paper, we have shown that if the relativity is taken into account and considerations are based on the Dirac rather than the Schrödinger or the Pauli equation for the electron, the leading term in the expansion of the induced electric quadrupole moment in powers of the field strength appears to be linear, not quadratic. The calculations of the actual value of that moment we have carried out in Sec. 4 provide a still another example of the usefulness of the Sturmian expansion of the generalized Dirac–Coulomb Green function [4] for analytical determination of electromagnetic properties of the relativistic one-electron atom.

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