PHYSICAL REVIEW A **85**, 042502 (2012)

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

Radosław Szmytkowski* and Patrycja Stefańska
Atomic Physics Division, Department of Atomic Physics and Luminescence, Faculty of Applied Physics and Mathematics, Gdańsk University of Technology, Narutowicza 11/12, 80–233 Gdańsk, Poland
(Received 7 November 2011; published 3 April 2012)

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 [Szmytkowski, J. Phys. B **30**, 825 (1997); **30**, 2747(E) (1997)], we derive a closed-form expression for an induced electric quadrupole moment. The result contains the generalized hypergeometric function ${}_3F_2$ of the unit argument. Earlier calculations by other authors, based on a nonrelativistic model of the atom, predicted in the low-field region the quadratic dependence of the induced electric quadrupole moment on B.

DOI: 10.1103/PhysRevA.85.042502 PACS number(s): 31.15.ap

I. INTRODUCTION

In the mid-1950s, Coulson and Stephen [1] pointed out that a uniform magnetic field should induce an electric quadrupole moment (EQM) in the hydrogenlike atom. They used the perturbation theory and found that in the case of the nonrelativistic 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. III) and to the notation used in the present work, is

$$\mathcal{Q}_{20} \simeq \mathcal{Q}_{20}^{(2)} = -\frac{5}{16}\frac{\alpha^4 e a_0^2}{Z^6}\frac{B^2}{B_0^2}, \tag{1.1}$$

where Ze is the nuclear charge, a_0 is the Bohr radius, α is the Sommerfeld fine-structure constant, and

$$B_0 = \frac{\mu_0}{4\pi}\frac{\mu_{\mathrm{B}}}{a_0^3} = \frac{\alpha^2\hbar}{2ea_0^2} \simeq 6.26\ \mathrm{T} \tag{1.2}$$

is the atomic unit of the magnetic induction (μ_0 is the vacuum permeability and μ_{B} is the Bohr magneton). Later, Turbiner [2] arrived at the same expression for $\mathcal{Q}_{20}^{(2)}$ for the Schrödinger one-electron atom with $Z = 1$ and found also explicitly the next nonvanishing term (being $\mathcal{Q}_{20}^{(4)} \propto B^4$) in the expansion of $\mathcal{Q}_{20}$ in powers of B. Moreover, using the variational technique, he determined the function $\mathcal{Q}_{20}(B)$ for magnetic fields ranging from vanishing to superstrong. A decade ago, Potekhin and Turbiner [3] calculated $\mathcal{Q}_{20}(B)$, 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] and the other 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 nonrelativistically. In the present paper, we show that if 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 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. IV we derive a closed-form expression for the induced EQM in terms of the generalized hypergeometric function ${}_3F_2$ with the unit argument.

II. 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 pointlike, infinitely heavy, and spinless and to carry the electric charge Ze. In the absence of external perturbations, the atomic ground-state energy level

$$E^{(0)} = mc^2\gamma_1, \tag{2.1}$$

where

$$\gamma_\kappa = \sqrt{\kappa^2 - (\alpha Z)^2}, \tag{2.2}$$

is twofold degenerate, with the two associated Hamiltonian eigenfunctions, orthonormal in the sense of

$$\int_{\mathbb{R}^3} d^3\boldsymbol{r}\, \Psi_\mu^{(0)\dagger}(\boldsymbol{r})\Psi_{\mu'}^{(0)}(\boldsymbol{r}) = \delta_{\mu\mu'}, \tag{2.3}$$

being

$$\Psi_\mu^{(0)}(\boldsymbol{r}) = \frac{1}{r}\begin{pmatrix} P^{(0)}(r)\Omega_{-1\mu}(\boldsymbol{n}_r) \\ iQ^{(0)}(r)\Omega_{1\mu}(\boldsymbol{n}_r)\end{pmatrix} \quad \left(\mu = \pm\tfrac{1}{2}\right). \tag{2.4}$$

*radek@mif.pg.gda.pl

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

$$\int_0^\infty dr\{[P^{(0)}(r)]^2 + [Q^{(0)}(r)]^2\} = 1, \tag{2.5}$$

are explicitly given by

$$P^{(0)}(r) = -\sqrt{\frac{Z}{a_0}\frac{1+\gamma_1}{\Gamma(2\gamma_1+1)}}\left(\frac{2Zr}{a_0}\right)^{\gamma_1} e^{-Zr/a_0}, \tag{2.6a}$$

$$Q^{(0)}(r) = \sqrt{\frac{Z}{a_0}\frac{1-\gamma_1}{\Gamma(2\gamma_1+1)}}\left(\frac{2Zr}{a_0}\right)^{\gamma_1} e^{-Zr/a_0}, \tag{2.6b}$$

whereas $\Omega_{\kappa\mu}(\boldsymbol{n}_r)$, with $\boldsymbol{n}_r = \boldsymbol{r}/r$, are the orthonormal spherical spinors defined as in Ref. [10].

In the presence of a weak, static, uniform magnetic field $\boldsymbol{B} = B\boldsymbol{n}_z$, the level $E^{(0)}$ splits in two. Their energies, to the first order in $\boldsymbol{B}$, are given by

$$E_\mu \simeq E^{(0)} + E_\mu^{(1)} \quad (\mu = \pm\tfrac{1}{2}), \tag{2.7}$$

with

$$E_\mu^{(1)} = \mathrm{sgn}(\mu)\frac{2\gamma_1+1}{3}\mu_{\mathrm{B}}B. \tag{2.8}$$

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

$$\Psi_\mu(\boldsymbol{r}) \simeq \Psi_\mu^{(0)}(\boldsymbol{r}) + \Psi_\mu^{(1)}(\boldsymbol{r}) \quad (\mu = \pm\tfrac{1}{2}). \tag{2.9}$$

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

$$\begin{aligned}\left[-ic\hbar\boldsymbol{\alpha}\cdot\nabla + \beta mc^2 - \frac{Ze^2}{(4\pi\epsilon_0)r} - E^{(0)}\right]\Psi_\mu^{(1)}(\boldsymbol{r})\\ = -\left[\frac{1}{2}ec\boldsymbol{\alpha}\cdot(\boldsymbol{B}\times\boldsymbol{r}) - E_\mu^{(1)}\right]\Psi_\mu^{(0)}(\boldsymbol{r})\end{aligned} \tag{2.10}$$

($\boldsymbol{\alpha}$ and β are the standard Dirac matrices), subject to the usual regularity conditions and the orthogonality constraint

$$\int_{\mathbb{R}^3} d^3\boldsymbol{r}\, \Psi_\mu^{(0)\dagger}(\boldsymbol{r})\Psi_{\mu'}^{(1)}(\boldsymbol{r}) = 0 \quad (\mu,\mu' = \pm\tfrac{1}{2}). \tag{2.11}$$

The integral representation of $\Psi_\mu^{(1)}(\boldsymbol{r})$ is

$$\Psi_\mu^{(1)}(\boldsymbol{r}) = -\frac{1}{2}ec\boldsymbol{B}\cdot\int_{\mathbb{R}^3} d^3\boldsymbol{r}'\, \bar{G}^{(0)}(\boldsymbol{r},\boldsymbol{r}')(\boldsymbol{r}'\times\boldsymbol{\alpha})\Psi_\mu^{(0)}(\boldsymbol{r}'), \tag{2.12}$$

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

III. 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 $\Psi_\mu(\boldsymbol{r})$? If $\rho_\mu(\boldsymbol{r})$ is the electronic charge density for that state, the spherical components of the Lth-order electric multipole moment tensor are defined as

$$\mathcal{Q}_{LM\mu} = \sqrt{\frac{4\pi}{2L+1}}\int_{\mathbb{R}^3} d^3\boldsymbol{r}\, r^L Y_{LM}^*(\boldsymbol{n}_r)\rho_\mu(\boldsymbol{r}), \tag{3.1}$$

where the asterisk denotes the complex conjugation and $Y_{LM}(\boldsymbol{n}_r)$ is the normalized spherical harmonic defined according to the Condon-Shortley phase convention [11]. For the atom in state $\Psi_\mu(\boldsymbol{r})$, the density $\rho_\mu(\boldsymbol{r})$ is given by

$$\rho_\mu(\boldsymbol{r}) = \frac{-e\Psi_\mu^\dagger(\boldsymbol{r})\Psi_\mu(\boldsymbol{r})}{\int_{\mathbb{R}^3} d^3\boldsymbol{r}'\, \Psi_\mu^\dagger(\boldsymbol{r}')\Psi_\mu(\boldsymbol{r}')}. \tag{3.2}$$

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

$$\rho_\mu(\boldsymbol{r}) \simeq \rho_\mu^{(0)}(\boldsymbol{r}) + \rho_\mu^{(1)}(\boldsymbol{r}), \tag{3.3}$$

with

$$\rho_\mu^{(0)}(\boldsymbol{r}) = -e\Psi_\mu^{(0)\dagger}(\boldsymbol{r})\Psi_\mu^{(0)}(\boldsymbol{r}) \tag{3.4}$$

and

$$\rho_\mu^{(1)}(\boldsymbol{r}) = -e\big[\Psi_\mu^{(1)\dagger}(\boldsymbol{r})\Psi_\mu^{(0)}(\boldsymbol{r}) + \Psi_\mu^{(0)\dagger}(\boldsymbol{r})\Psi_\mu^{(1)}(\boldsymbol{r})\big]. \tag{3.5}$$

Accordingly, it follows that

$$\mathcal{Q}_{LM\mu} \simeq \mathcal{Q}_{LM\mu}^{(0)} + \mathcal{Q}_{LM\mu}^{(1)}, \tag{3.6}$$

where

$$\mathcal{Q}_{LM\mu}^{(0)} = -e\sqrt{\frac{4\pi}{2L+1}}\int_{\mathbb{R}^3} d^3\boldsymbol{r}\, \Psi_\mu^{(0)\dagger}(\boldsymbol{r})r^L Y_{LM}^*(\boldsymbol{n}_r)\Psi_\mu^{(0)}(\boldsymbol{r}) \tag{3.7}$$

is the multipole moment for the unperturbed atom, and

$$\mathcal{Q}_{LM\mu}^{(1)} = \widetilde{\mathcal{Q}}_{LM\mu}^{(1)} + (-1)^M\widetilde{\mathcal{Q}}_{L,-M\mu}^{(1)*}, \tag{3.8}$$

with

$$\widetilde{\mathcal{Q}}_{LM\mu}^{(1)} = -e\sqrt{\frac{4\pi}{2L+1}}\int_{\mathbb{R}^3} d^3\boldsymbol{r}\, \Psi_\mu^{(0)\dagger}(\boldsymbol{r})r^L Y_{LM}^*(\boldsymbol{n}_r)\Psi_\mu^{(1)}(\boldsymbol{r}), \tag{3.9}$$

is the first-order correction induced by the perturbing magnetic field. To arrive at Eq. (3.8), we have exploited the well-known identity

$$Y_{LM}(\boldsymbol{n}_r) = (-1)^M Y_{L,-M}^*(\boldsymbol{n}_r). \tag{3.10}$$

If the representation (2.12) of $\Psi_\mu^{(1)}(\boldsymbol{r})$ is plugged into Eq. (3.9), it gives $\widetilde{\mathcal{Q}}_{LM\mu}^{(1)}$ in the form of the double integral over $\mathbb{R}^3$:

$$\begin{aligned}\widetilde{\mathcal{Q}}_{LM\mu}^{(1)} = \frac{1}{2}\sqrt{\frac{4\pi}{2L+1}}\, e^2cB\\ \times\int_{\mathbb{R}^3} d^3\boldsymbol{r}\int_{\mathbb{R}^3} d^3\boldsymbol{r}'\, \Psi_\mu^{(0)\dagger}(\boldsymbol{r})r^L Y_{LM}^*(\boldsymbol{n}_r)\bar{G}^{(0)}(\boldsymbol{r},\boldsymbol{r}')\boldsymbol{n}_z\\ \cdot(\boldsymbol{r}'\times\boldsymbol{\alpha})\Psi_\mu^{(0)}(\boldsymbol{r}').\end{aligned} \tag{3.11}$$

Using Eq. (2.4) and the explicit representations of the spherical spinors $\Omega_{\mp1\mu}(\boldsymbol{n}_r)$, it is easy to show that the electronic charge density in the unperturbed atom $\rho_\mu^{(0)}(\boldsymbol{r})$ 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

$$\mathcal{Q}^{(0)}_{LM\mu} = -e\delta_{L0}\delta_{M0}, \tag{3.12}$$

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 $\mathcal{Q}^{(1)}_{LM\mu}$. To this end, we have to invoke the multipole representation of the generalized Green function, which is

$$\bar{G}^{(0)}(\boldsymbol{r},\boldsymbol{r}') = \frac{4\pi\epsilon_0}{e^2}\sum_{\substack{\kappa=-\infty\\(\kappa\neq 0)}}^{\infty}\sum_{m=-|\kappa|+1/2}^{|\kappa|-1/2}\frac{1}{rr'}\begin{pmatrix} \bar{g}^{(0)}_{\kappa,(++)}(r,r')\Omega_{\kappa m}(\boldsymbol{n}_r)\Omega^{\dagger}_{\kappa m}(\boldsymbol{n}'_r) & -i\,\bar{g}^{(0)}_{\kappa,(+-)}(r,r')\Omega_{\kappa m}(\boldsymbol{n}_r)\Omega^{\dagger}_{-\kappa m}(\boldsymbol{n}'_r) \\ i\,\bar{g}^{(0)}_{\kappa,(-+)}(r,r')\Omega_{-\kappa m}(\boldsymbol{n}_r)\Omega^{\dagger}_{\kappa m}(\boldsymbol{n}'_r) & \bar{g}^{(0)}_{\kappa,(--)}(r,r')\Omega_{-\kappa m}(\boldsymbol{n}_r)\Omega^{\dagger}_{-\kappa m}(\boldsymbol{n}'_r)\end{pmatrix}. \tag{3.13}$$

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 [see [10], Eq. (3.1.6)]

$$\boldsymbol{n}_z\cdot(\boldsymbol{n}_r\times\boldsymbol{\sigma})\,\Omega_{\kappa\mu}(\boldsymbol{n}_r) = i\,\frac{4\mu\kappa}{4\kappa^2-1}\Omega_{-\kappa\mu}(\boldsymbol{n}_r) + i\,\frac{\sqrt{\left(\kappa+\frac{1}{2}\right)^2-\mu^2}}{|2\kappa+1|}\Omega_{\kappa+1,\mu}(\boldsymbol{n}_r) - i\,\frac{\sqrt{\left(\kappa-\frac{1}{2}\right)^2-\mu^2}}{|2\kappa-1|}\Omega_{\kappa-1,\mu}(\boldsymbol{n}_r) \tag{3.14}$$

and the relation

$$\sqrt{\frac{4\pi}{2L+1}}\oint_{4\pi} d^2\boldsymbol{n}_r\,\Omega^{\dagger}_{\kappa\mu}(\boldsymbol{n}_r)Y^{*}_{LM}(\boldsymbol{n}_r)\Omega_{\kappa'\mu'}(\boldsymbol{n}_r) = (-1)^{\mu'+1/2}2\sqrt{|\kappa\kappa'|}\begin{pmatrix}|\kappa|-\frac{1}{2} & L & |\kappa'|-\frac{1}{2}\\ -\frac{1}{2} & 0 & \frac{1}{2}\end{pmatrix} \times\begin{pmatrix}|\kappa|-\frac{1}{2} & L & |\kappa'|-\frac{1}{2}\\ \mu & M & -\mu'\end{pmatrix}\Pi(l,L,l'), \tag{3.15}$$

with

$$\Pi(l,L,l') = \begin{cases}1 & \text{for} \quad l+L+l' \text{ even}\\ 0 & \text{for} \quad l+L+l' \text{ odd.}\end{cases} \tag{3.16}$$

In Eq. (3.15), $\left(\begin{smallmatrix} j_a & j_b & j_c\\ m_a & m_b & m_c\end{smallmatrix}\right)$ denotes Wigner's $3j$ coefficient, whereas

$$l = \left|\kappa+\tfrac{1}{2}\right| - \tfrac{1}{2} \tag{3.17}$$

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 $\widetilde{\mathcal{Q}}^{(1)}_{LM\mu}$ does not vanish is the one with $L=2$ and $M=0$. Since $\widetilde{\mathcal{Q}}^{(1)}_{20\mu}$ is real, from Eq. (3.8) one has

$$\mathcal{Q}^{(1)}_{LM\mu} = \mathcal{Q}^{(1)}_{20\mu}\delta_{L2}\delta_{M0}, \tag{3.18}$$

with $\mathcal{Q}^{(1)}_{20\mu}$ being given in the form of the following double radial integral:

$$\mathcal{Q}^{(1)}_{20\mu} = \mathrm{sgn}(\mu)\frac{2}{15}(4\pi\epsilon_0)cB\int_0^{\infty}dr\int_0^{\infty}dr'\,(P^{(0)}(r)\quad Q^{(0)}(r)) \times r^2\bar{\mathsf{G}}^{(0)}_2(r,r')r'\begin{pmatrix}Q^{(0)}(r')\\ P^{(0)}(r')\end{pmatrix}, \tag{3.19}$$

where

$$\bar{\mathsf{G}}^{(0)}_{\kappa}(r,r') = \begin{pmatrix}\bar{g}^{(0)}_{\kappa,(++)}(r,r') & \bar{g}^{(0)}_{\kappa,(+-)}(r,r')\\ \bar{g}^{(0)}_{\kappa,(-+)}(r,r') & \bar{g}^{(0)}_{\kappa,(--)}(r,r')\end{pmatrix} \tag{3.20}$$

is the radial generalized Green function.

IV. 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 nonvanishing spherical component is the one with $M=0$. Now, the Cartesian components of the traceless tensor of the induced quadrupole moment,

$$\mathcal{Q}^{(1)}_{ij\mu} = \int_{\mathbb{R}^3} d^3\boldsymbol{r}\,\frac{1}{2}(3r_ir_j - r^2\delta_{ij})\rho^{(1)}_{\mu}(\boldsymbol{r}) \quad (i,j\in\{x,y,z\}), \tag{4.1}$$

are related to its spherical components through

$$\begin{pmatrix}\mathcal{Q}^{(1)}_{xx\mu} & \mathcal{Q}^{(1)}_{xy\mu} & \mathcal{Q}^{(1)}_{xz\mu}\\ \mathcal{Q}^{(1)}_{yx\mu} & \mathcal{Q}^{(1)}_{yy\mu} & \mathcal{Q}^{(1)}_{yz\mu}\\ \mathcal{Q}^{(1)}_{zx\mu} & \mathcal{Q}^{(1)}_{zy\mu} & \mathcal{Q}^{(1)}_{zz\mu}\end{pmatrix} = \begin{pmatrix} -\frac{1}{2}\mathcal{Q}^{(1)}_{20\mu} + \sqrt{\frac{3}{8}}\left[\mathcal{Q}^{(1)}_{22\mu} + \mathcal{Q}^{(1)}_{2-2\mu}\right] & i\sqrt{\frac{3}{8}}\left[\mathcal{Q}^{(1)}_{22\mu} - \mathcal{Q}^{(1)}_{2-2\mu}\right] & -\sqrt{\frac{3}{8}}\left[\mathcal{Q}^{(1)}_{21\mu} - \mathcal{Q}^{(1)}_{2-1\mu}\right]\\ i\sqrt{\frac{3}{8}}\left[\mathcal{Q}^{(1)}_{22\mu} - \mathcal{Q}^{(1)}_{2-2\mu}\right] & -\frac{1}{2}\mathcal{Q}^{(1)}_{20\mu} - \sqrt{\frac{3}{8}}\left[\mathcal{Q}^{(1)}_{22\mu} + \mathcal{Q}^{(1)}_{2-2\mu}\right] & -i\sqrt{\frac{3}{8}}\left[\mathcal{Q}^{(1)}_{21\mu} + \mathcal{Q}^{(1)}_{2-1\mu}\right]\\ -\sqrt{\frac{3}{8}}\left[\mathcal{Q}^{(1)}_{21\mu} - \mathcal{Q}^{(1)}_{2-1\mu}\right] & -i\sqrt{\frac{3}{8}}\left[\mathcal{Q}^{(1)}_{21\mu} + \mathcal{Q}^{(1)}_{2-1\mu}\right] & \mathcal{Q}^{(1)}_{20\mu}\end{pmatrix}. \tag{4.2}$$

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:

$$\mathcal{Q}_{ij\mu}^{(1)} = 0 \quad (i \neq j;\, i,j \in \{x,y,z\}), \tag{4.3}$$

while the diagonal elements are given by

$$\mathcal{Q}_{xx\mu}^{(1)} = \mathcal{Q}_{yy\mu}^{(1)} = -\tfrac{1}{2}\mathcal{Q}_{zz\mu}^{(1)} = -\tfrac{1}{2}\mathcal{Q}_{20\mu}^{(1)}. \tag{4.4}$$

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]

$$\bar{\mathsf{G}}_{\kappa}^{(0)}(r,r') = \sum_{n_r=-\infty}^{\infty} \frac{1}{\mu_{n_r\kappa}^{(0)} - 1} \begin{pmatrix} S_{n_r\kappa}^{(0)}(r) \\ T_{n_r\kappa}^{(0)}(r) \end{pmatrix} \times \left(\mu_{n_r\kappa}^{(0)} S_{n_r\kappa}^{(0)}(r') \;\; T_{n_r\kappa}^{(0)}(r') \right) \quad (\kappa \neq -1) \tag{4.5}$$

[the formula in Eq. (4.5) remains valid in the case of $\kappa = 1$ because there is no $1p_{1/2}$ hydrogenic energy level degenerate with the actual $1s_{1/2}$ one; for details, see Ref. [4]]. Here

$$S_{n_r\kappa}^{(0)}(r) = \sqrt{\frac{(1+\gamma_1)(|n_r|+2\gamma_\kappa)|n_r|!}{2ZN_{n_r\kappa}\left(N_{n_r\kappa}-\kappa\right)\Gamma(|n_r|+2\gamma_\kappa)}} \left(\frac{2Zr}{a_0}\right)^{\gamma_\kappa} e^{-Zr/a_0} \times \left[L_{|n_r|-1}^{(2\gamma_\kappa)}\left(\frac{2Zr}{a_0}\right) + \frac{\kappa - N_{n_r\kappa}}{|n_r|+2\gamma_\kappa} L_{|n_r|}^{(2\gamma_\kappa)}\left(\frac{2Zr}{a_0}\right) \right] \tag{4.6a}$$

and

$$T_{n_r\kappa}^{(0)}(r) = \sqrt{\frac{(1-\gamma_1)(|n_r|+2\gamma_\kappa)|n_r|!}{2ZN_{n_r\kappa}\left(N_{n_r\kappa}-\kappa\right)\Gamma(|n_r|+2\gamma_\kappa)}} \left(\frac{2Zr}{a_0}\right)^{\gamma_\kappa} e^{-Zr/a_0} \times \left[L_{|n_r|-1}^{(2\gamma_\kappa)}\left(\frac{2Zr}{a_0}\right) - \frac{\kappa - N_{n_r\kappa}}{|n_r|+2\gamma_\kappa} L_{|n_r|}^{(2\gamma_\kappa)}\left(\frac{2Zr}{a_0}\right) \right] \tag{4.6b}$$

[with $L_n^{(\alpha)}(\rho)$ denoting the generalized Laguerre polynomial [12]; we define $L_{-1}^{(\alpha)}(\rho) \equiv 0$] are the radial Dirac-Coulomb Sturmian functions associated with the hydrogenic ground-state energy level, and

$$\mu_{n_r\kappa}^{(0)} = \frac{|n_r| + \gamma_\kappa + N_{n_r\kappa}}{\gamma_1 + 1}, \tag{4.7}$$

with

$$N_{n_r\kappa} = \pm\sqrt{(|n_r|+\gamma_\kappa)^2 + (\alpha Z)^2} = \pm\sqrt{|n_r|^2 + 2|n_r|\gamma_\kappa + \kappa^2} \tag{4.8}$$

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 sign 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 $\mathcal{Q}_{20\mu}^{(1)}$:

$$\mathcal{Q}_{20\mu}^{(1)} = \operatorname{sgn}(\mu)\frac{2}{15}(4\pi\epsilon_0)cB \sum_{n_r=-\infty}^{\infty} \frac{1}{\mu_{n_r2}^{(0)} - 1} \times \int_0^\infty dr\, r^2\left[P^{(0)}(r)S_{n_r2}^{(0)}(r) + Q^{(0)}(r)T_{n_r2}^{(0)}(r)\right] \times \int_0^\infty dr'\, r'\left[\mu_{n_r2}^{(0)}Q^{(0)}(r')S_{n_r2}^{(0)}(r') + P^{(0)}(r')T_{n_r2}^{(0)}(r')\right]. \tag{4.9}$$

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 $S_{n_r2}^{(0)}(r)$, $T_{n_r2}^{(0)}(r)$, given by Eqs. (2.6) and (4.6), respectively. Exploiting the known integral formula [see [13], Eq. (7.414.11)]

$$\int_0^\infty dx\, x^\gamma e^{-x} L_n^{(\alpha)}(x) = \frac{\Gamma(\gamma+1)\Gamma(n+\alpha-\gamma)}{n!\,\Gamma(\alpha-\gamma)} \quad [\mathrm{Re}(\gamma) > -1] \tag{4.10}$$

and the trivial but extremely useful identity

$$\gamma_2^2 = \gamma_1^2 + 3, \tag{4.11}$$

one arrives at

$$\mathcal{Q}_{20\mu}^{(1)} = -\operatorname{sgn}(\mu)\frac{\alpha^2 e a_0^2}{Z^4}\frac{B}{B_0}\frac{\Gamma^2(\gamma_1+\gamma_2+3)}{480(4\gamma_1+1)\Gamma(2\gamma_1+1)\Gamma^2(\gamma_2-\gamma_1-2)} \times \sum_{n_r=-\infty}^{\infty} \frac{\Gamma(|n_r|+\gamma_2-\gamma_1-3)\Gamma(|n_r|+\gamma_2-\gamma_1-2)}{|n_r|!\,\Gamma(|n_r|+2\gamma_2+1)}\frac{N_{n_r2}-2}{N_{n_r2}} \times \frac{(|n_r|+\gamma_2-3\gamma_1-3-\gamma_1N_{n_r2})(3|n_r|+\gamma_1+3\gamma_2+1+3N_{n_r2})}{|n_r|+\gamma_2-\gamma_1-1+N_{n_r2}}. \tag{4.12}$$

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

$$\mathcal{Q}^{(1)}_{20\mu} = \mathrm{sgn}(\mu)\frac{\alpha^2 e a_0^2}{Z^4}\frac{B}{B_0}\frac{\Gamma^2(\gamma_1+\gamma_2+3)}{240(4\gamma_1+1)\Gamma(2\gamma_1+1)\Gamma^2(\gamma_2-\gamma_1-2)}\sum_{n_r=0}^{\infty}\frac{\Gamma(n_r+\gamma_2-\gamma_1-3)\Gamma(n_r+\gamma_2-\gamma_1-2)}{n_r!(n_r+\gamma_2-\gamma_1)\Gamma(n_r+2\gamma_2+1)}$$
$$\times[(2\gamma_1-1)(n_r+\gamma_2-\gamma_1-3)(n_r+\gamma_2-\gamma_1)+2(\gamma_1+1)(2\gamma_1+1)(n_r+\gamma_2-\gamma_1)-6(\gamma_1+1)]. \tag{4.13}$$

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

$$\sum_{n=0}^{\infty}\frac{\Gamma(n+a_1)\Gamma(n+a_2)}{n!\Gamma(n+b)} = \frac{\Gamma(a_1)\Gamma(a_2)}{\Gamma(b)}\,{}_2F_1\left(\begin{matrix}a_1,a_2\\ b\end{matrix};1\right) \tag{4.14}$$

and

$$\sum_{n=0}^{\infty}\frac{\Gamma(n+a_1)\Gamma(n+a_2)}{n!(n+a_3)\Gamma(n+b)} = \frac{\Gamma(a_1)\Gamma(a_2)}{a_3\Gamma(b)}\,{}_3F_2\left(\begin{matrix}a_1,a_2,a_3\\ a_3+1,b\end{matrix};1\right), \tag{4.15}$$

Eq. (4.13) becomes

$$\mathcal{Q}^{(1)}_{20\mu} = -\,\mathrm{sgn}(\mu)\frac{\alpha^2 e a_0^2}{Z^4}\frac{B}{B_0}\frac{\Gamma(\gamma_1+\gamma_2+3)\Gamma(\gamma_1+\gamma_2+4)}{1440(\gamma_1+1)(4\gamma_1+1)\Gamma(2\gamma_1+1)\Gamma(2\gamma_2+1)}$$
$$\times\left[(2\gamma_1-1)(\gamma_2-\gamma_1-3)\,{}_2F_1\left(\begin{matrix}\gamma_2-\gamma_1-2,\gamma_2-\gamma_1-2\\ 2\gamma_2+1\end{matrix};1\right)\right.$$
$$+2(\gamma_1+1)(2\gamma_1+1)\,{}_2F_1\left(\begin{matrix}\gamma_2-\gamma_1-3,\gamma_2-\gamma_1-2\\ 2\gamma_2+1\end{matrix};1\right)$$
$$\left.-\frac{6(\gamma_1+1)}{\gamma_2-\gamma_1}\,{}_3F_2\left(\begin{matrix}\gamma_2-\gamma_1-3,\gamma_2-\gamma_1-2,\gamma_2-\gamma_1\\ \gamma_2-\gamma_1+1,2\gamma_2+1\end{matrix};1\right)\right]. \tag{4.16}$$

The two ${}_2F_1$ functions may be then eliminated with the aid of the Gauss identity [Ref. [13], Eq. (9.122.1)]

$${}_2F_1\left(\begin{matrix}a_1,a_2\\ b\end{matrix};1\right) = \frac{\Gamma(b)\Gamma(b-a_1-a_2)}{\Gamma(b-a_1)\Gamma(b-a_2)} \quad [\mathrm{Re}(b-a_1-a_2)>0]. \tag{4.17}$$

After some simple algebra, we obtain

$$\mathcal{Q}^{(1)}_{20\mu} = \mathrm{sgn}(\mu)\frac{\alpha^2 e a_0^2}{Z^4}\frac{B}{B_0}\frac{\Gamma(2\gamma_1+5)}{720(4\gamma_1+1)\Gamma(2\gamma_1+1)}\left[-2\left(2\gamma_1^2+3\gamma_1+4\right)+\frac{(\gamma_1+\gamma_2)\Gamma(\gamma_1+\gamma_2+3)\Gamma(\gamma_1+\gamma_2+4)}{\Gamma(2\gamma_1+5)\Gamma(2\gamma_2+1)}\right.$$
$$\left.\times\,{}_3F_2\left(\begin{matrix}\gamma_2-\gamma_1-3,\gamma_2-\gamma_1-2,\gamma_2-\gamma_1\\ \gamma_2-\gamma_1+1,2\gamma_2+1\end{matrix};1\right)\right]. \tag{4.18}$$

Various other equivalent representations of $\mathcal{Q}^{(1)}_{20\mu}$ 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

$${}_3F_2\left(\begin{matrix}a_1,a_2,a_3\\ a_3+1,b\end{matrix};1\right) = -\frac{a_3}{a_1-a_3}\frac{\Gamma(b)\Gamma(b-a_1-a_2)}{\Gamma(b-a_1)\Gamma(b-a_2)}+\frac{a_1}{a_1-a_3}\,{}_3F_2\left(\begin{matrix}a_1+1,a_2,a_3\\ a_3+1,b\end{matrix};1\right) \quad [\mathrm{Re}(b-a_1-a_2)>0] \tag{4.19}$$

and its analog with a_1 and a_2 interchanged, Eq. (4.18) is transformed into the slightly more compact expression

$$\mathcal{Q}^{(1)}_{20\mu} = \mathrm{sgn}(\mu)\frac{\alpha^2 e a_0^2}{Z^4}\frac{B}{B_0}\frac{\Gamma(2\gamma_1+5)}{1440\,\Gamma(2\gamma_1)}\left[-1+\frac{(\gamma_1+1)(\gamma_1+\gamma_2)\Gamma(\gamma_1+\gamma_2+2)\Gamma(\gamma_1+\gamma_2+3)}{\gamma_1\Gamma(2\gamma_1+5)\Gamma(2\gamma_2+1)}\right.$$
$$\left.\times\,{}_3F_2\left(\begin{matrix}\gamma_2-\gamma_1-2,\gamma_2-\gamma_1-1,\gamma_2-\gamma_1\\ \gamma_2-\gamma_1+1,2\gamma_2+1\end{matrix};1\right)\right]. \tag{4.20}$$

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

$$\gamma_\kappa \simeq |\kappa| - \frac{(\alpha Z)^2}{2|\kappa|} \quad (\kappa \in \mathbb{Z}\setminus\{0\}), \tag{4.21}$$

and consequently,

$$\Gamma(\gamma_\kappa + \gamma_{\kappa'} + k) \simeq (|\kappa| + |\kappa'| + k - 1)!\left[1 - \frac{1}{2}\left(\frac{1}{|\kappa|} + \frac{1}{|\kappa'|}\right)\psi\left(|\kappa| + |\kappa'| + k\right)(\alpha Z)^2\right] \quad (\kappa,\kappa' \in \mathbb{Z} \setminus \{0\}, k \in \mathbb{N}), \tag{4.22}$$

where

$$\psi(\zeta) = \frac{1}{\Gamma(\zeta)}\frac{d\Gamma(\zeta)}{d\zeta} \tag{4.23}$$

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

$$\psi(\zeta + 1) = \psi(\zeta) + \frac{1}{\zeta} \tag{4.24}$$

yields

$$\frac{(\gamma_1 + 1)(\gamma_1 + \gamma_2)\Gamma(\gamma_1 + \gamma_2 + 2)\Gamma(\gamma_1 + \gamma_2 + 3)}{\gamma_1\Gamma(2\gamma_1 + 5)\Gamma(2\gamma_2 + 1)} \simeq 1 + \frac{13}{60}(\alpha Z)^2. \tag{4.25}$$

Since, at the same time, to the second order in αZ, it holds that

$${}_3F_2\left(\begin{matrix}\gamma_2 - \gamma_1 - 2, \gamma_2 - \gamma_1 - 1, \gamma_2 - \gamma_1 \\ \gamma_2 - \gamma_1 + 1, 2\gamma_2 + 1\end{matrix}; 1\right) \simeq 1 - \frac{(\alpha Z)^2}{40}, \tag{4.26}$$

the sought approximation to $\mathcal{Q}^{(1)}_{20\mu}$ is

$$\mathcal{Q}^{(1)}_{20\mu} \simeq \mathrm{sgn}(\mu)\frac{23}{240}\frac{\alpha^4 e a_0^2}{Z^2}\frac{B}{B_0} \quad (\alpha Z \ll 1). \tag{4.27}$$

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

V. CONCLUSIONS

Earlier calculations of the magnetic field-induced electric quadrupole moment in the ground state of the hydrogenlike atom, based on the nonrelativistic 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 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 that we have carried out in Sec. IV provide 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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