Static magnetic multipole susceptibilities of the relativistic hydrogenlike atom in the ground state: Application of the Sturmian expansion of the generalized Dirac-Coulomb Green function

Radosław Szmytkowski* and Grzegorz Łukasik

Atomic and Optical Physics Division, Department of Atomic, Molecular and Optical Physics, Faculty of Applied Physics and Mathematics, Gdańsk University of Technology, ul. Gabriela Narutowicza 11/12, 80–233 Gdańsk, Poland

(Received 17 April 2018; published 8 August 2018)

We study far- and near-field magnetic and electric multipole moments induced in the ground state of the Dirac one-electron atom placed in a weak 2^L-pole magnetostatic field. The analysis is carried out within the framework of the first-order Rayleigh-Schrödinger perturbation theory, with the use of the Sturmian expansion of the generalized Dirac-Coulomb Green function [Szmytkowski, J. Phys. B **30**, 825 (1997); **30**, 2747(E) (1997)]. Closed-form analytical expressions for multipole magnetizabilities χ_L, magnetic nuclear shielding constants $\sigma_{\mathrm{M}L\to\mathrm{M}L}$, the far-field magnetic-to-electric cross-susceptibilities $\chi_{\mathrm{M}L\to\mathrm{E}(L\mp1)}$, and the near-field counterparts $\sigma_{\mathrm{M}L\to\mathrm{E}(L\mp1)}$ of the latter are derived. The formulas obtained for χ_L and $\sigma_{\mathrm{M}L\to\mathrm{M}L}$ are much simpler than those available in the literature. We establish the relationship $\chi_{\mathrm{M}L\to\mathrm{E}(L\mp1)} = \alpha_{\mathrm{E}(L\mp1)\to\mathrm{M}L}$, where $\alpha_{\mathrm{E}(L\mp1)\to\mathrm{M}L}$ are the multipole far-field electric-to-magnetic susceptibilities discussed in our previous paper [Szmytkowski and Łukasik, Phys. Rev. A **93**, 062502 (2016)]. It is also found that when the atom is placed in superimposed weak and static electric and magnetic fields of respective multipolarities 2^{L_1} and 2^{L_2}, such that $L_1 = L_2 \mp 1$, then the second-order correction to the ground-state energy contains an additional term entangling both fields and involving the cross-susceptibility $\alpha_{\mathrm{E}L_1\to\mathrm{M}L_2} = \chi_{\mathrm{M}L_2\to\mathrm{E}L_1}$.

DOI: 10.1103/PhysRevA.98.022502

I. INTRODUCTION

In a series of papers published over the past years, our group presented applications of the Sturmian expansion of the Dirac-Coulomb Green function [1] in perturbative calculations of various kinds of electric and magnetic susceptibilities for relativistic hydrogenic ions in the ground [2–11] and excited [12–17] states. In those works, it was assumed that perturbing fields, either electric or magnetic, were of the dipolar nature. An exception has been the recent work [10], in which we have dealt with the general electric multipolar case. In the latter paper, we have derived analytical expressions for atomic ground-state multipole polarizabilities α_L, electric nuclear shielding constants $\sigma_{\mathrm{E}L\to\mathrm{E}L}$, far- and near-field electric-to-magnetic cross-susceptibilities $\alpha_{\mathrm{E}L\to\mathrm{M}(L\mp1)}$ and $\sigma_{\mathrm{E}L\to\mathrm{M}(L\mp1)}$, and also for far- and near-field electric-to-toroidal-magnetic cross-susceptibilities $\alpha_{\mathrm{E}L\to\mathrm{T}L}$ and $\sigma_{\mathrm{E}L\to\mathrm{T}L}$. In the current paper, which is a natural complement to Ref. [10], we shall be concerned with magnetostatic multipole susceptibilities of the Dirac one-electron atom[1] in the ground state. Specifically, we shall investigate multipole magnetizabilities χ_L, magnetic nuclear shielding constants $\sigma_{\mathrm{M}L\to\mathrm{M}L}$, the far-field magnetic-to-electric cross-susceptibilities $\chi_{\mathrm{M}L\to\mathrm{E}(L\mp1)}$, and also their near-field counterparts $\sigma_{\mathrm{M}L\to\mathrm{E}(L\mp1)}$.

Our search through the literature has revealed only two earlier papers, in which an effect of relativity on hydrogenic magnetic susceptibilities was studied in the general multipolar case. In Ref. [18], Manakov *et al.* used a series expansion of the Dirac-Coulomb Green function in a Sturmian basis associated with the second-order Dirac-Coulomb equation, and expressed the ground-state multipole susceptibilities χ_L in terms of four nonterminating generalized hypergeometric functions ${}_3F_2(1)$ with the unit argument. The same mathematical tool was exploited by that group in Ref. [19], where the ground-state multipole magnetic nuclear shielding constants $\sigma_{\mathrm{M}L\to\mathrm{M}L}$ were obtained in a form involving four finite sums, each one being related to a truncating ${}_3F_2(1)$ function. The results from Refs. [18,19] were recounted in the monograph [20, Sec. 4.6]. The reason for which we have decided to report in the current paper our formulas for the susceptibilities χ_L and $\sigma_{\mathrm{M}L\to\mathrm{M}L}$ is that they appear to be much simpler than those presented in Refs. [18,19]; each of our expressions contains only two, rather than four, generalized hypergeometric functions ${}_3F_2(1)$. As concerns the cross-susceptibilities $\chi_{\mathrm{M}L\to\mathrm{E}\lambda}$ and $\sigma_{\mathrm{M}L\to\mathrm{E}\lambda}$, which characterize an electric response of the atom perturbed by an external 2^L-pole magnetic field, it seems they have not been subjects of studies thus far.

The paper is structured as follows. In Sec. II, we shall present a mathematical model, based on the Dirac-Coulomb equation, for the one-electron atom in the ground state placed in a weak 2^L-pole magnetostatic field. In Sec. III, we shall carry out a detailed analysis of the far-field multipole magnetic moments induced in the atom by the field and derive expressions for related multipole magnetizabilities χ_L. In Sec. IV, we shall show that a 2^L-pole magnetic field induces in the atom only far-field electric multipole moments of orders $2^{L\mp1}$, and then we shall prove that pertinent magnetic-to-electric cross-susceptibilities $\chi_{\mathrm{M}L\to\mathrm{E}(L\mp1)}$ are related to their

*Corresponding author: Radoslaw.Szmytkowski@pg.edu.pl

[1] Throughout this work, the term "atom" is used in the broad sense and refers both to the genuine hydrogen atom (with $Z = 1$) as well as to hydrogenlike ions (with $Z \geqslant 2$).

electric-to-magnetic counterparts $\alpha_{\mathrm{E}(L\mp1)\to\mathrm{M}L}$ from Ref. [10] through the identity $\chi_{\mathrm{M}L\to\mathrm{E}(L\mp1)} = \alpha_{\mathrm{E}(L\mp1)\to\mathrm{M}L}$. Multipole magnetic nuclear shielding constants $\sigma_{\mathrm{M}L\to\mathrm{M}L}$ and the near-field cross-susceptibilities $\sigma_{\mathrm{M}L\to\mathrm{E}(L\mp1)}$ will be determined in Secs. V and VI, respectively, from the analysis of induced near-field magnetic and electric multipole moments. (In Secs. IV–VI we shall be brief and shall omit details of calculations which, to a large extent, parallel those from Sec. III.) A summary and concluding remarks will form Sec. VII. In Appendix A, we shall list several formulas for multiple (triple, quadruple, and quintuple) sums over magnetic quantum numbers which have proved to be useful for evaluation of angular integrals appearing in Secs. III–VI and those from Appendixes B and C. In Appendix B, we shall relate the multipole magnetizability χ_L to the second-order correction to energy for the atom in the 2^L-pole magnetic field. The resulting formula may serve as a definition of the magnetizability χ_L, alternative, but still equivalent, to the one which appears in Sec. III. Finally, in Appendix C we shall show that if the atom is placed in a combination of two fields, an electrostatic one of multipolarity 2^{L_1} and a magnetostatic one of multipolarity 2^{L_2}, such that $L_1 = L_2 \mp 1$, then the second-order correction to the atomic ground-state energy includes a term which entangles both fields and contains the far-field cross-susceptibility $\chi_{\mathrm{M}L_2\to\mathrm{E}L_1} = \alpha_{\mathrm{E}L_1\to\mathrm{M}L_2}$. This proves that the cross-susceptibilities are measurable quantities.

II. PRELIMINARIES

The system we shall be concerned with in the present work is a Dirac one-electron atom with a motionless and pointlike nucleus. We shall be assuming that the only nonvanishing electromagnetic moment characterizing the nucleus is its electric charge equal to $+Ze$. The position vector of an atomic electron with respect to the nucleus will be denoted as $\boldsymbol{r}$ and the unit vector in that direction as $\boldsymbol{n}_r$. The atom is placed in an external static 2^L-pole magnetic field of induction $\boldsymbol{\mathcal{B}}_L^{(1)}(\boldsymbol{r})$, which may be derived, with the aid of the relation $\boldsymbol{\mathcal{B}}_L^{(1)}(\boldsymbol{r}) = \nabla \times \boldsymbol{\mathcal{A}}_L^{(1)}(\boldsymbol{r})$, from the vector potential

$$\boldsymbol{\mathcal{A}}_L^{(1)}(\boldsymbol{r}) = -i\sqrt{\frac{4\pi L}{(L+1)(2L+1)}}\, r^L \times \sum_{M=-L}^{L} \mathcal{D}_{LM}^{(1)*} \boldsymbol{Y}_{LM}^{L}(\boldsymbol{n}_r) \quad (L \geqslant 1) \tag{2.1}$$

(the asterisk denotes the complex conjugation); the field $\boldsymbol{\mathcal{B}}_L^{(1)}(\boldsymbol{r})$ is

$$\boldsymbol{\mathcal{B}}_L^{(1)}(\boldsymbol{r}) = \sqrt{4\pi L}\, r^{L-1} \sum_{M=-L}^{L} \mathcal{D}_{LM}^{(1)*} \boldsymbol{Y}_{LM}^{L-1}(\boldsymbol{n}_r) \quad (L \geqslant 1). \tag{2.2}$$

The coefficients $\mathcal{D}_{LM}^{(1)}$, constrained to obey

$$\mathcal{D}_{LM}^{(1)*} = (-)^M \mathcal{D}_{L,-M}^{(1)}, \tag{2.3}$$

are components of a spherical tensor operator $\mathsf{D}_L^{(1)}$ of rank L, while $\boldsymbol{Y}_{LM}^{L'}(\boldsymbol{n}_r)$ are the vector spherical harmonics [21, Sec. 7.3]; in particular, one has

$$\boldsymbol{Y}_{LM}^{L}(\boldsymbol{n}_r) = \frac{\boldsymbol{\Lambda} Y_{LM}(\boldsymbol{n}_r)}{\sqrt{L(L+1)}}, \tag{2.4}$$

where $\boldsymbol{\Lambda} = -i\boldsymbol{r} \times \nabla$, while $Y_{LM}(\boldsymbol{n}_r)$ are the scalar spherical harmonics normalized in accordance with the Condon-Shortley convention. Since it holds that

$$\boldsymbol{Y}_{LM}^{L*}(\boldsymbol{n}_r) = (-)^{M+1} \boldsymbol{Y}_{L,-M}^{L}(\boldsymbol{n}_r), \tag{2.5}$$

the relation (2.3) guarantees that the vector potential (2.1) is real, and so is the magnetic field (2.2). Observe that for $L = 1$ the coefficients $\mathcal{D}_{1M}^{(1)}$ are simply cyclic components of the spatially uniform magnetic field $\boldsymbol{\mathcal{B}}_1^{(1)} = \mathcal{B}_1^{(1)}\boldsymbol{n}$ (with $\mathcal{B}_1^{(1)} = |\boldsymbol{\mathcal{B}}_1^{(1)}|$), i.e., one has

$$\mathcal{D}_{1M}^{(1)} = \mathcal{B}_{1M}^{(1)} \quad (M = 0, \pm 1). \tag{2.6}$$

The Dirac equation describing the bound atomic electron subjected both to the Coulombic force due to the nucleus and the Lorentz force due to the external magnetic field is

$$\left[-ic\hbar\boldsymbol{\alpha}\cdot\nabla + \beta m_{\mathrm{e}}c^2 - \frac{Ze^2}{(4\pi\epsilon_0)r} + V_L^{(1)}(\boldsymbol{r}) - E\right]\Psi(\boldsymbol{r}) = 0, \tag{2.7}$$

where $\boldsymbol{\alpha}$ and β are the standard Dirac matrices, while

$$\begin{aligned} V_L^{(1)}(\boldsymbol{r}) &= ec\boldsymbol{\alpha}\cdot\boldsymbol{\mathcal{A}}_L^{(1)}(\boldsymbol{r}) \\ &= -iec\sqrt{\frac{4\pi L}{(L+1)(2L+1)}}\, r^L \\ &\quad \times \sum_{M=-L}^{L} \mathcal{D}_{LM}^{(1)*} \boldsymbol{\alpha}\cdot\boldsymbol{Y}_{LM}^{L}(\boldsymbol{n}_r) \quad (L \geqslant 1) \end{aligned} \tag{2.8}$$

is the electron–magnetic-field interaction energy. Equation (2.7) must be solved subject to the standard regularity and boundary conditions, the latter being of the form

$$\lim_{r\to0} r\Psi(\boldsymbol{r}) = 0, \quad \lim_{r\to\infty} r^{3/2}\Psi(\boldsymbol{r}) = 0, \tag{2.9}$$

imposed on the electronic spinor wave function $\Psi(\boldsymbol{r})$.

Throughout the rest of this paper, we shall focus on the *ground-state* properties of the atom described by the Dirac equation (2.7) in the case when the magnetic field is so weak that the operator (2.8) is a small perturbation of a Dirac-Coulomb Hamiltonian of an isolated atom. Then, to the first order in the perturbation, we approximate the ground-state eigenenergy E as

$$E \simeq E^{(0)} + E^{(1)}, \tag{2.10}$$

where $E^{(0)}$ is the ground-state energy of an isolated atom, given by

$$E^{(0)} = m_{\mathrm{e}}c^2\gamma_1, \tag{2.11}$$

with

$$\gamma_\kappa = \sqrt{\kappa^2 - (\alpha Z)^2} \tag{2.12}$$

(here and below α, which should not be confused with the Dirac matrix $\boldsymbol{\alpha}$, denotes the Sommerfeld fine-structure constant). The value of the first-order energy correction $E^{(1)}$ will be determined below. In the same manner, we approximate the ground-state wave function as

$$\Psi(\boldsymbol{r}) \simeq \Psi^{(0)}(\boldsymbol{r}) + \Psi^{(1)}(\boldsymbol{r}), \tag{2.13}$$

where $\Psi^{(0)}(\boldsymbol{r})$ stands for the perturbation-adapted wave function of the isolated atom in its ground state. It is of the form

$$\Psi^{(0)}(\boldsymbol{r}) = a_{1/2}\Psi^{(0)}_{1/2}(\boldsymbol{r}) + a_{-1/2}\Psi^{(0)}_{-1/2}(\boldsymbol{r}), \tag{2.14}$$

where

$$\Psi^{(0)}_{m}(\boldsymbol{r}) = \frac{1}{r}\begin{pmatrix} P^{(0)}(r)\Omega_{-1m}(\boldsymbol{n}_r) \\ iQ^{(0)}(r)\Omega_{1m}(\boldsymbol{n}_r) \end{pmatrix} \quad \left(m = \pm\frac{1}{2}\right), \tag{2.15}$$

with the radial functions given by

$$P^{(0)}(r) = -\sqrt{\frac{Z}{a_0}\frac{1+\gamma_1}{\Gamma(2\gamma_1+1)}}\left(\frac{2Zr}{a_0}\right)^{\gamma_1} e^{-Zr/a_0}, \tag{2.16a}$$

$$Q^{(0)}(r) = \sqrt{\frac{Z}{a_0}\frac{1-\gamma_1}{\Gamma(2\gamma_1+1)}}\left(\frac{2Zr}{a_0}\right)^{\gamma_1} e^{-Zr/a_0} \tag{2.16b}$$

(a_0 is the Bohr radius) and with $\Omega_{\kappa m}(\boldsymbol{n}_r)$ being the spherical spinors [22]. The functions (2.15) are orthonormal in the sense of

$$\int_{\mathbb{R}^3} d^3\boldsymbol{r}\; \Psi^{(0)\dagger}_{m}(\boldsymbol{r})\Psi^{(0)}_{m'}(\boldsymbol{r}) = \delta_{mm'} \quad \left(m,m' = \pm\frac{1}{2}\right), \tag{2.17}$$

and if the normalization constraint

$$\int_{\mathbb{R}^3} d^3\boldsymbol{r}\; \Psi^{(0)\dagger}(\boldsymbol{r})\Psi^{(0)}(\boldsymbol{r}) = 1 \tag{2.18}$$

is set, this restricts the coefficients $a_{\pm 1/2}$ to obey

$$|a_{1/2}|^2 + |a_{-1/2}|^2 = 1. \tag{2.19}$$

Proceeding along the standard route of the Rayleigh-Schrödinger perturbation theory, one finds that the correction $\Psi^{(1)}(\boldsymbol{r})$ solves the inhomogeneous equation

$$\left[-ic\hbar\boldsymbol{\alpha}\cdot\nabla + \beta m_{\mathrm{e}}c^2 - \frac{Ze^2}{(4\pi\epsilon_0)r} - E^{(0)}\right]\Psi^{(1)}(\boldsymbol{r}) = -\left[V^{(1)}_{L}(\boldsymbol{r}) - E^{(1)}\right]\Psi^{(0)}(\boldsymbol{r}), \tag{2.20}$$

under the same conditions which have been imposed before on solutions to Eq. (2.7), and also subject to the additional orthogonality restraint

$$\int_{\mathbb{R}^3} d^3\boldsymbol{r}\; \Psi^{(0)\dagger}_{m}(\boldsymbol{r})\Psi^{(1)}(\boldsymbol{r}) = 0 \quad \left(m = \pm\frac{1}{2}\right). \tag{2.21}$$

Insertion of Eq. (2.14) into the right-hand side of Eq. (2.20), followed by projection of the resulting equation onto the unperturbed eigenfunctions $\Psi^{(0)}_{m}(\boldsymbol{r})$, leads to the following algebraic system for the coefficients $a_{\pm 1/2}$:

$$\sum_{m'=-1/2}^{1/2}\left[V^{(1)}_{L,mm'} - E^{(1)}\delta_{mm'}\right]a_{m'} = 0 \quad \left(m = \pm\frac{1}{2}\right), \tag{2.22}$$

where

$$V^{(1)}_{L,mm'} = -iec\sqrt{\frac{4\pi L}{(L+1)(2L+1)}}\sum_{M=-L}^{L}\mathcal{D}^{(1)*}_{LM} \times \int_{\mathbb{R}^3} d^3\boldsymbol{r}\,\Psi^{(0)\dagger}_{m}(\boldsymbol{r})r^L\boldsymbol{\alpha}\cdot\boldsymbol{Y}^{L}_{LM}(\boldsymbol{n}_r)\Psi^{(0)}_{m'}(\boldsymbol{r}). \tag{2.23}$$

Adopting, for the sake of brevity, the bracket notation

$$\langle\Omega_{\kappa m_\kappa}|\hat{O}\Omega_{\kappa' m_{\kappa'}}\rangle \equiv \oint_{4\pi} d^2\boldsymbol{n}_r\;\Omega^{\dagger}_{\kappa m_\kappa}(\boldsymbol{n}_r)\hat{O}\Omega_{\kappa' m_{\kappa'}}(\boldsymbol{n}_r), \tag{2.24}$$

with the aid of the identities

$$\langle\Omega_{\kappa m}|\boldsymbol{\sigma}\cdot\boldsymbol{Y}^{L}_{LM}\Omega_{\kappa' m'}\rangle = \frac{\kappa'-\kappa}{\sqrt{L(L+1)}}\langle\Omega_{\kappa m}|Y_{LM}\Omega_{\kappa' m'}\rangle \tag{2.25}$$

and

$$\langle\Omega_{-\kappa m}|Y_{LM}\Omega_{-\kappa' m'}\rangle = \langle\Omega_{\kappa m}|Y_{LM}\Omega_{\kappa' m'}\rangle, \tag{2.26}$$

the matrix element in Eq. (2.23) may be cast into the form

$$V^{(1)}_{L,mm'} = \frac{4ec}{L+1}\sqrt{\frac{4\pi}{2L+1}}\int_0^\infty dr\, r^L P^{(0)}(r)Q^{(0)}(r) \times \sum_{M=-L}^{L}\mathcal{D}^{(1)*}_{LM}\langle\Omega_{-1m}|Y_{LM}\Omega_{1m'}\rangle. \tag{2.27}$$

Using then the well-known formula

$$\sqrt{\frac{4\pi}{2L+1}}\langle\Omega_{\kappa m_\kappa}|Y_{LM}\Omega_{\kappa' m_{\kappa'}}\rangle = (-)^{m_\kappa+1/2}2\sqrt{|\kappa\kappa'|}\begin{pmatrix}|\kappa|-\frac{1}{2} & L & |\kappa'|-\frac{1}{2}\\ -\frac{1}{2} & 0 & \frac{1}{2}\end{pmatrix} \times \begin{pmatrix}|\kappa|-\frac{1}{2} & L & |\kappa'|-\frac{1}{2}\\ m_\kappa & -M & -m_{\kappa'}\end{pmatrix}\Pi(l_\kappa,L,l_{\kappa'}), \tag{2.28}$$

where $\begin{pmatrix}j_a & j_b & j_c\\ m_a & m_b & m_c\end{pmatrix}$ denotes the Wigner's $3j$ coefficient, while

$$\Pi(l_\kappa,L,l_{\kappa'}) = \begin{cases}1 & \text{for } l_\kappa+L+l_{\kappa'} \text{ even}\\ 0 & \text{for } l_\kappa+L+l_{\kappa'} \text{ odd,}\end{cases} \tag{2.29}$$

with

$$l_\kappa = \left|\kappa+\tfrac{1}{2}\right| - \tfrac{1}{2}, \tag{2.30}$$

one finds that

$$\langle\Omega_{-1m}|Y_{LM}\Omega_{1m'}\rangle = \frac{\delta_{L1}}{\sqrt{4\pi}}\left[\sqrt{\frac{2}{3}}\,\delta_{M1}\delta_{m,1/2}\delta_{m',-1/2} - \frac{1}{\sqrt{3}}\delta_{M0}(\delta_{m,1/2}\delta_{m',1/2} - \delta_{m,-1/2}\delta_{m',-1/2}) - \sqrt{\frac{2}{3}}\,\delta_{M,-1}\delta_{m,-1/2}\delta_{m',1/2}\right]. \tag{2.31}$$

The Kronecker delta δ_{L1} appearing in the above formula causes that the cases $L = 1$ and $L \geqslant 2$ have to be considered separately.

At first, let $L = 1$, when the perturbing magnetic field $\boldsymbol{\mathcal{B}}^{(1)}_1 = \mathbf{D}^{(1)}_1$ is spatially uniform. Inserting Eq. (2.31) and the result

$$\int_0^\infty dr\, r P^{(0)}(r) Q^{(0)}(r) = -\alpha a_0 \frac{1}{4}(2\gamma_1 + 1) \tag{2.32}$$

into Eq. (2.25) yields the elements $V^{(1)}_{1,mm'}$, which may be arranged in the Hermitian matrix

$$\mathsf{V}^{(1)}_1 = \begin{pmatrix} V^{(1)}_{1,1/2,1/2} & V^{(1)}_{1,1/2,-1/2} \\ V^{(1)}_{1,-1/2,1/2} & V^{(1)}_{1,-1/2,-1/2} \end{pmatrix} = \frac{1}{3}(2\gamma_1 + 1)\mu_{\mathrm{B}} \begin{pmatrix} \mathcal{D}^{(1)}_{10} & \sqrt{2}\,\mathcal{D}^{(1)}_{1,-1} \\ -\sqrt{2}\,\mathcal{D}^{(1)}_{11} & -\mathcal{D}^{(1)}_{10} \end{pmatrix}, \tag{2.33}$$

where

$$\mu_{\mathrm{B}} = \frac{e\hbar}{2m_{\mathrm{e}}} \tag{2.34}$$

is the Bohr magneton. From Eq. (2.33) one easily deduces that two eigenvalues of $\mathsf{V}^{(1)}_1$, i.e., the first-order energy corrections $E^{(1)}$ to $E^{(0)}$, are

$$E^{(1)}_\pm = \pm\tfrac{1}{3}(2\gamma_1 + 1)\mu_{\mathrm{B}}\left|\mathbf{D}^{(1)}_1\right| \quad (L = 1), \tag{2.35}$$

where

$$\left|\mathbf{D}^{(1)}_1\right| = \sqrt{\mathcal{D}^{(1)2}_{10} - 2\mathcal{D}^{(1)}_{11}\mathcal{D}^{(1)}_{1,-1}} = \sqrt{\mathcal{D}^{(1)2}_{10} + 2\left|\mathcal{D}^{(1)}_{11}\right|^2} \tag{2.36}$$

is the modulus of the magnetic induction vector $\boldsymbol{\mathcal{B}}^{(1)}_1 = \mathbf{D}^{(1)}_1$. Let $0 \leqslant \vartheta_1 \leqslant \pi$ and $0 \leqslant \phi_1 < 2\pi$ be spherical angles such that

$$\mathcal{D}^{(1)}_{10} = \left|\mathbf{D}^{(1)}_1\right| \cos\vartheta_1, \quad \mathcal{D}^{(1)}_{1,\pm1} = \mp\frac{1}{\sqrt{2}}\left|\mathbf{D}^{(1)}_1\right| e^{\pm i\phi_1} \sin\vartheta_1. \tag{2.37}$$

Then from Eqs. (2.22), (2.33), and (2.35), we have

$$\frac{a_{1/2}}{a_{-1/2}} = -\frac{\sqrt{2}\,\mathcal{D}^{(1)}_{1,-1}}{\mathcal{D}^{(1)}_{10} \mp \left|\mathbf{D}^{(1)}_1\right|} = e^{-i\phi_\pm} \cot\frac{\vartheta_\pm}{2} \quad (E^{(1)} = E^{(1)}_\pm), \tag{2.38}$$

where

$$\vartheta_+ = \vartheta_1, \quad \phi_+ = \phi_1 \tag{2.39a}$$

and

$$\vartheta_- = \pi - \vartheta_1, \quad \phi_- = \phi_1 \pm \pi \quad \text{for} \quad \phi_1 \lesseqgtr \pi. \tag{2.39b}$$

Hence, after the constraint (2.19) is taken into account, it follows that for $L = 1$ the mixing coefficients in Eq. (2.14) may be chosen to be

$$a_{1/2} = e^{-i(\chi_\pm + \phi_\pm)/2} \cos\frac{\vartheta_\pm}{2}, \quad a_{-1/2} = e^{-i(\chi_\pm - \phi_\pm)/2} \sin\frac{\vartheta_\pm}{2} \quad (E^{(1)} = E^{(1)}_\pm), \tag{2.40}$$

with $0 \leqslant \chi_\pm < 4\pi$. In what follows, whenever the case $L = 1$ is considered, perturbation-adjusted zeroth-order wave functions with the coefficients (2.40) will be denoted as $\Psi^{(0)}_\pm(\boldsymbol{r})$.

The case of $L \geqslant 2$ is much simpler, since then the angular integral (2.31) is zero, and so is the right-hand side of Eq. (2.27):

$$V^{(1)}_{L,mm'} = 0 \quad (L \geqslant 2). \tag{2.41}$$

Consequently, we see from Eq. (2.22) that, to the first order in the perturbation, the multipole magnetic fields with $L \geqslant 2$ do not shift the atomic ground-state energy level:

$$E^{(1)} = 0 \quad (L \geqslant 2), \tag{2.42}$$

and that the mixing coefficients $a_{\pm1/2}$ in Eq. (2.14) may be chosen freely.

Whatever L is, once the coefficients $a_{\pm1/2}$, and thus the perturbation-adapted zeroth-order wave function $\Psi^{(0)}(\boldsymbol{r})$, are known, the corresponding first-order correction $\Psi^{(1)}(\boldsymbol{r})$ to the latter may be obtained from the formula

$$\Psi^{(1)}(\boldsymbol{r}) = iec\sqrt{\frac{4\pi L}{(L+1)(2L+1)}} \sum_{M=-L}^{L} \mathcal{D}^{(1)*}_{LM} \times \int_{\mathbb{R}^3} d^3\boldsymbol{r}'\, \bar{G}^{(0)}(\boldsymbol{r},\boldsymbol{r}') r'^L \boldsymbol{\alpha} \cdot \boldsymbol{Y}^L_{LM}(\boldsymbol{n}'_r) \Psi^{(0)}(\boldsymbol{r}'). \tag{2.43}$$

Here $\bar{G}^{(0)}(\boldsymbol{r},\boldsymbol{r}')$ is the generalized Dirac-Coulomb Green function associated with the ground-state energy level (2.11) of the Dirac-Coulomb Hamiltonian (cf. Ref. [1, Sec. 4]). It may be represented by the multipole expansion

$$\bar{G}^{(0)}(\boldsymbol{r},\boldsymbol{r}') = \frac{4\pi\epsilon_0}{e^2} \sum_{\substack{\kappa=-\infty \\ (\kappa\neq0)}}^{\infty} \sum_{m_\kappa=-|\kappa|+1/2}^{|\kappa|-1/2} \frac{1}{rr'} \begin{pmatrix} \bar{g}^{(0)}_{(++)\kappa}(r,r')\Omega_{\kappa m_\kappa}(\boldsymbol{n}_r)\Omega^\dagger_{\kappa m_\kappa}(\boldsymbol{n}'_r) & -i\,\bar{g}^{(0)}_{(+-)\kappa}(r,r')\Omega_{\kappa m_\kappa}(\boldsymbol{n}_r)\Omega^\dagger_{-\kappa m_\kappa}(\boldsymbol{n}'_r) \\ i\,\bar{g}^{(0)}_{(-+)\kappa}(r,r')\Omega_{-\kappa m_\kappa}(\boldsymbol{n}_r)\Omega^\dagger_{\kappa m_\kappa}(\boldsymbol{n}'_r) & \bar{g}^{(0)}_{(--)\kappa}(r,r')\Omega_{-\kappa m_\kappa}(\boldsymbol{n}_r)\Omega^\dagger_{-\kappa m_\kappa}(\boldsymbol{n}'_r) \end{pmatrix}. \tag{2.44}$$

The four radial functions $\bar{g}^{(0)}_{(\pm\pm)\kappa}(r,r')$ appearing herein may be collected into the 2×2 matrix

$$\bar{\mathsf{G}}^{(0)}_\kappa(r,r') = \begin{pmatrix} \bar{g}^{(0)}_{(++)\kappa}(r,r') & \bar{g}^{(0)}_{(+-)\kappa}(r,r') \\ \bar{g}^{(0)}_{(-+)\kappa}(r,r') & \bar{g}^{(0)}_{(--)\kappa}(r,r') \end{pmatrix}, \tag{2.45}$$

which forms the radial generalized Dirac-Coulomb Green function for the atomic ground state. Depending on whether $\kappa \neq -1$ or $\kappa = -1$, the latter may be given in the forms of the following Sturmian series expansions:

$$\bar{\mathsf{G}}^{(0)}_\kappa(r,r') = \sum_{n_r=-\infty}^{\infty} \frac{1}{\mu^{(0)}_{n_r\kappa} - 1} \begin{pmatrix} S^{(0)}_{n_r\kappa}(r) \\ T^{(0)}_{n_r\kappa}(r) \end{pmatrix} \begin{pmatrix} \mu^{(0)}_{n_r\kappa} S^{(0)}_{n_r\kappa}(r') & T^{(0)}_{n_r\kappa}(r') \end{pmatrix} \quad (\kappa \neq -1) \tag{2.46}$$

and

$$\bar{\mathsf{G}}^{(0)}_{-1}(r,r') = \sum_{\substack{n_r=-\infty \\ (n_r\neq 0)}}^{\infty} \frac{1}{\mu^{(0)}_{n_r,-1}-1} \begin{pmatrix} S^{(0)}_{n_r,-1}(r) \\ T^{(0)}_{n_r,-1}(r) \end{pmatrix} \left(\mu^{(0)}_{n_r,-1} S^{(0)}_{n_r,-1}(r') \quad T^{(0)}_{n_r,-1}(r')\right) + \left(\gamma_1 - \frac{1}{2}\right) \begin{pmatrix} S^{(0)}_{0,-1}(r) \\ T^{(0)}_{0,-1}(r) \end{pmatrix} \left(S^{(0)}_{0,-1}(r') \quad T^{(0)}_{0,-1}(r')\right)$$
$$+ \begin{pmatrix} I_{0,-1}(r) \\ K_{0,-1}(r) \end{pmatrix} \left(S^{(0)}_{0,-1}(r') \quad T^{(0)}_{0,-1}(r')\right) + \begin{pmatrix} S^{(0)}_{0,-1}(r) \\ T^{(0)}_{0,-1}(r) \end{pmatrix} \left(J_{0,-1}(r') \quad K_{0,-1}(r')\right), \tag{2.47}$$

in the latter case with

$$I_{0,-1}(r) = \gamma_1 r \frac{dS^{(0)}_{0,-1}(r)}{\mathrm{d}r} - \frac{1}{2} S^{(0)}_{0,-1}(r), \tag{2.48a}$$

$$J_{0,-1}(r) = \gamma_1 r \frac{dS^{(0)}_{0,-1}(r)}{\mathrm{d}r} + \frac{1}{2} S^{(0)}_{0,-1}(r), \tag{2.48b}$$

and

$$K_{0,-1}(r) = \gamma_1 r \frac{dT^{(0)}_{0,-1}(r)}{\mathrm{d}r} + \frac{1}{2} T^{(0)}_{0,-1}(r). \tag{2.48c}$$

The functions $S^{(0)}_{n_r\kappa}(r)$ and $T^{(0)}_{n_r\kappa}(r)$, appearing in Eqs. (2.46)–(2.48), are the radial Dirac-Coulomb Sturmian functions associated with the ground state of the atom. Their explicit representations are

$$S^{(0)}_{n_r\kappa}(r) = \sqrt{\frac{(1+\gamma_1)(|n_r|+2\gamma_\kappa)|n_r|!}{2ZN_{n_r\kappa}(N_{n_r\kappa}-\kappa)\Gamma(|n_r|+2\gamma_\kappa)}} \left(\frac{2Zr}{a_0}\right)^{\gamma_\kappa} e^{-Zr/a_0} \left[L^{(2\gamma_\kappa)}_{|n_r|-1}\left(\frac{2Zr}{a_0}\right) + \frac{\kappa - N_{n_r\kappa}}{|n_r|+2\gamma_\kappa} L^{(2\gamma_\kappa)}_{|n_r|}\left(\frac{2Zr}{a_0}\right)\right] \tag{2.49a}$$

and

$$T^{(0)}_{n_r\kappa}(r) = \sqrt{\frac{(1-\gamma_1)(|n_r|+2\gamma_\kappa)|n_r|!}{2ZN_{n_r\kappa}(N_{n_r\kappa}-\kappa)\Gamma(|n_r|+2\gamma_\kappa)}} \left(\frac{2Zr}{a_0}\right)^{\gamma_\kappa} e^{-Zr/a_0} \left[L^{(2\gamma_\kappa)}_{|n_r|-1}\left(\frac{2Zr}{a_0}\right) - \frac{\kappa - N_{n_r\kappa}}{|n_r|+2\gamma_\kappa} L^{(2\gamma_\kappa)}_{|n_r|}\left(\frac{2Zr}{a_0}\right)\right], \tag{2.49b}$$

where $L^{(\alpha)}_n(\rho)$ denotes the generalized Laguerre polynomial [23]; we define $L^{(\alpha)}_{-1}(\rho) \equiv 0$. The parameter $N_{n_r\kappa}$ is a Sturmian "apparent" principal quantum number defined as

$$\begin{aligned} N_{n_r\kappa} &= \pm\sqrt{(|n_r|+\gamma_\kappa)^2 + (\alpha Z)^2} \\ &= \pm\sqrt{|n_r|^2 + 2|n_r|\gamma_\kappa + \kappa^2}, \end{aligned} \tag{2.50}$$

with the convention that the plus sign is to 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 $\kappa > 0$, i.e., one has $N_{0\kappa} = -\kappa$. It is easy to verify that in the particular case of $n_r = 0$ and $\kappa = -1$ it holds that

$$S^{(0)}_{0,-1}(r) = \frac{\sqrt{a_0}}{Z} P^{(0)}(r), \quad T^{(0)}_{0,-1}(r) = \frac{\sqrt{a_0}}{Z} Q^{(0)}(r). \tag{2.51}$$

Finally, the parameter $\mu^{(0)}_{n_r\kappa}$ entering Eqs. (2.46) and (2.47) is a Sturmian eigenvalue given by

$$\mu^{(0)}_{n_r\kappa} = \frac{|n_r| + \gamma_\kappa + N_{n_r\kappa}}{\gamma_1 + 1}. \tag{2.52}$$

III. MAGNETIC MULTIPOLE MOMENTS OF THE ATOM IN THE MULTIPOLE MAGNETIC FIELD AND ATOMIC MULTIPOLE MAGNETIZABILITIES

A. Decomposition of the atomic magnetic multipole moments into the permanent and the first-order magnetic-field-induced components

In magnetostatics, spherical components of the 2^λ-pole magnetic moment M_λ of a system of sourceless electric currents characterized by the distribution $\boldsymbol{j}(\boldsymbol{r})$ are defined as [10, Appendix B]

$$\mathcal{M}_{\lambda\mu} = -i\sqrt{\frac{4\pi\lambda}{(\lambda+1)(2\lambda+1)}} \int_{\mathbb{R}^3} d^3\boldsymbol{r}\, r^\lambda \boldsymbol{Y}^\lambda_{\lambda\mu}(\boldsymbol{n}_r) \cdot \boldsymbol{j}(\boldsymbol{r}), \tag{3.1}$$

with $\mu = 0, \pm1, \ldots, \pm\lambda$. In the case of an atom in the magnetic field investigated in this work, the current density $\boldsymbol{j}(\boldsymbol{r})$ in the electronic cloud is given by

$$\boldsymbol{j}(\boldsymbol{r}) = \frac{-ec\Psi^\dagger(\boldsymbol{r})\boldsymbol{\alpha}\Psi(\boldsymbol{r})}{\int_{\mathbb{R}^3} d^3\boldsymbol{r}'\, \Psi^\dagger(\boldsymbol{r}')\Psi(\boldsymbol{r}')}, \tag{3.2}$$

where the spinor wave function $\Psi(\boldsymbol{r})$ solves Eq. (2.7). Under the assumptions given in Sec. II, with the aid of Eqs. (2.13), (2.18), and (2.21), the current density (3.2) may be approximated as

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

where

$$\boldsymbol{j}^{(0)}(\boldsymbol{r}) = -ec\Psi^{(0)\dagger}(\boldsymbol{r})\boldsymbol{\alpha}\Psi^{(0)}(\boldsymbol{r}) \tag{3.4}$$

is the current density in an isolated atom, while

$$\boldsymbol{j}^{(1)}(\boldsymbol{r}) = -2ec\,\mathrm{Re}[\Psi^{(0)\dagger}(\boldsymbol{r})\boldsymbol{\alpha}\Psi^{(1)}(\boldsymbol{r})] \tag{3.5}$$

is the first-order field-induced correction to the latter. Accordingly, one has

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

where

$$\mathcal{M}_{\lambda\mu}^{(0)} = -i\sqrt{\frac{4\pi\lambda}{(\lambda+1)(2\lambda+1)}}\int_{\mathbb{R}^3} d^3\boldsymbol{r}\, r^{\lambda}\boldsymbol{Y}_{\lambda\mu}^{\lambda}(\boldsymbol{n}_r)\cdot\boldsymbol{j}^{(0)}(\boldsymbol{r}) \tag{3.7}$$

are components of the 2^{λ}-pole moment $\mathbf{M}_{\lambda}^{(0)}$ of an unperturbed atom, while the set of $2\lambda+1$ quantities

$$\mathcal{M}_{\lambda\mu}^{(1)} = -i\sqrt{\frac{4\pi\lambda}{(\lambda+1)(2\lambda+1)}}\int_{\mathbb{R}^3} d^3\boldsymbol{r}\, r^{\lambda}\boldsymbol{Y}_{\lambda\mu}^{\lambda}(\boldsymbol{n}_r)\cdot\boldsymbol{j}^{(1)}(\boldsymbol{r}) \tag{3.8}$$

defines the first-order 2^{λ}-pole field-induced moment $\mathbf{M}_{\lambda}^{(1)}$.

The unperturbed moments $\mathbf{M}_{\lambda}^{(0)}$ have been considered in Ref. [9], where it has been shown that the only nonvanishing magnetic moment of an isolated atom is the dipole one:

$$\mathbf{M}_{\lambda}^{(0)} = \mathbf{M}_{\lambda}^{(0)}\delta_{\lambda 1}. \tag{3.9}$$

The cyclic components of $\mathbf{M}_{1}^{(0)}$, expressed in terms of the superposition coefficients $a_{\pm 1/2}$ appearing in Eq. (2.14), are given by

$$\mathcal{M}_{1,0}^{(0)} = -\frac{1}{3}(2\gamma_1+1)\mu_{\mathrm{B}}(|a_{1/2}|^2 - |a_{-1/2}|^2), \tag{3.10a}$$

$$\mathcal{M}_{1,\pm 1}^{(0)} = \pm\frac{\sqrt{2}}{3}(2\gamma_1+1)\mu_{\mathrm{B}}a_{\pm 1/2}^{*}a_{\mp 1/2}. \tag{3.10b}$$

If the unit vector $\boldsymbol{\nu}$, with the spherical components

$$\nu_0 = |a_{1/2}|^2 - |a_{-1/2}|^2, \quad \nu_{\pm 1} = \mp\sqrt{2}\,a_{\pm 1/2}^{*}a_{\mp 1/2}, \tag{3.11}$$

is introduced, Eqs. (3.10a) and (3.10b) may be compactly rewritten as

$$\mathbf{M}_{1}^{(0)} = -\frac{2\gamma_1+1}{3}\mu_{\mathrm{B}}\boldsymbol{\nu}. \tag{3.12}$$

The parametrization

$$\begin{aligned} a_{1/2} &= e^{-i(\chi+\phi)/2}\cos\frac{\vartheta}{2}, \\ a_{-1/2} &= e^{-i(\chi-\phi)/2}\sin\frac{\vartheta}{2} \\ &\quad (0 \leqslant \chi < 4\pi,\ 0 \leqslant \phi < 2\pi,\ 0 \leqslant \vartheta \leqslant \pi), \end{aligned} \tag{3.13}$$

admitted by the normalization constraint (2.19) for arbitrary $L \geqslant 1$ [obviously, for $L = 1$ the angles ϑ, φ, and χ in the above formula are the angles $\vartheta_{\pm}$, $\phi_{\pm}$, and $\chi_{\pm}$ from Eq. (2.39)], casts the two formulas in Eq. (3.11) into

$$\nu_0 = \cos\vartheta, \quad \nu_{\pm 1} = \mp\frac{1}{\sqrt{2}}e^{\pm i\phi}\sin\vartheta, \tag{3.14}$$

i.e., ϑ and ϕ are, respectively, the polar and the azimuthal angles of the vector $\boldsymbol{\nu}$ in the spherical system of coordinates. It follows from Eqs. (3.14), (2.37), and (2.39) that for $L = 1$ the vector $\boldsymbol{\nu}$ is either parallel or antiparallel to the perturbing field $\boldsymbol{\mathcal{B}}_{1}^{(1)} = \mathbf{D}_{1}^{(1)}$, depending on whether the resulting first-order energy correction $E^{(1)}$ [cf. Eq. (2.35)] is positive or negative.

We next proceed to the analysis of the induced moments. Insertion of Eq. (3.5) into Eq. (3.8) gives

$$\mathcal{M}_{\lambda\mu}^{(1)} = \widetilde{\mathcal{M}}_{\lambda\mu}^{(1)} + (-)^{\mu}\widetilde{\mathcal{M}}_{\lambda,-\mu}^{(1)*}, \tag{3.15}$$

where

$$\widetilde{\mathcal{M}}_{\lambda\mu}^{(1)} = iec\sqrt{\frac{4\pi\lambda}{(\lambda+1)(2\lambda+1)}} \times \int_{\mathbb{R}^3} d^3\boldsymbol{r}\,\Psi^{(0)\dagger}(\boldsymbol{r})r^{\lambda}\boldsymbol{\alpha}\cdot\boldsymbol{Y}_{\lambda\mu}^{\lambda}(\boldsymbol{n}_r)\Psi^{(1)}(\boldsymbol{r}). \tag{3.16}$$

Use of Eq. (2.43) transforms Eq. (3.16) into

$$\widetilde{\mathcal{M}}_{\lambda\mu}^{(1)} = -4\pi e^2c^2\sqrt{\frac{\lambda L}{(\lambda+1)(2\lambda+1)(L+1)(2L+1)}} \times \sum_{M=-L}^{L}\mathcal{D}_{LM}^{(1)*}\int_{\mathbb{R}^3} d^3\boldsymbol{r}\int_{\mathbb{R}^3} d^3\boldsymbol{r}'\,\Psi^{(0)\dagger}(\boldsymbol{r})r^{\lambda}\boldsymbol{\alpha}\cdot\boldsymbol{Y}_{\lambda\mu}^{\lambda}(\boldsymbol{n}_r)\bar{G}^{(0)}(\boldsymbol{r},\boldsymbol{r}')r'^{L}\boldsymbol{\alpha}\cdot\boldsymbol{Y}_{LM}^{L}(\boldsymbol{n}_r')\Psi^{(0)}(\boldsymbol{r}'). \tag{3.17}$$

To evaluate the double integral in Eq. (3.17), we insert into it the representation of $\Psi^{(0)}(\boldsymbol{r})$ which follows from Eqs. (2.14) and (2.15), and then replace the generalized Green function $\bar{G}^{(0)}(\boldsymbol{r},\boldsymbol{r}')$ by its multipole expansion (2.44). This enables one to perform integrations over angular and radial variables separately. Using the identities (2.25) and (2.26), we obtain

$$\widetilde{\mathcal{M}}_{\lambda\mu}^{(1)} = \left(\frac{\mu_0}{4\pi}\right)^{-1}\frac{4\pi}{(\lambda+1)(L+1)\sqrt{(2\lambda+1)(2L+1)}}\sum_{\substack{\kappa=-\infty \\ (\kappa\neq 0)}}^{\infty}(\kappa-1)^2R_{\kappa}^{(\lambda,L)}(Q^{(0)},P^{(0)};Q^{(0)},P^{(0)}) \times \sum_{M=-L}^{L}\sum_{m=-1/2}^{1/2}\sum_{m'=-1/2}^{1/2}\sum_{m_\kappa=-|\kappa|+1/2}^{|\kappa|-1/2}\mathcal{D}_{LM}^{(1)*}a_m^{*}a_{m'}\langle\Omega_{-1m}|Y_{\lambda\mu}\Omega_{-\kappa m_\kappa}\rangle\langle\Omega_{-\kappa m_\kappa}|Y_{LM}\Omega_{-1m'}\rangle. \tag{3.18}$$

Here $R_{\kappa}^{(\lambda,L)}(Q^{(0)},P^{(0)};Q^{(0)},P^{(0)})$ is a particular case of the general double radial integral

$$R_{\kappa}^{(L_1,L_2)}(F_a,F_b;F_c,F_d)=\int_0^{\infty}dr\int_0^{\infty}dr'(F_a(r)\ \ F_b(r))r^{L_1}\bar{\mathsf{G}}_{\kappa}^{(0)}(r,r')r'^{L_2}\begin{pmatrix}F_c(r')\\F_d(r')\end{pmatrix}, \tag{3.19}$$

with $\bar{\mathsf{G}}_{\kappa}^{(0)}(r,r')$ standing for the radial generalized Dirac-Coulomb Green function (2.45). The quadruple sum over M, m, m', and m_κ appearing in Eq. (3.18) is akin to the one in Eq. (A10). Hence, we find that

$$\widetilde{\mathcal{M}}_{\lambda\mu}^{(1)}=\widetilde{\mathcal{M}}_{\lambda\mu}^{(1)}\delta_{\lambda L}, \tag{3.20}$$

where

$$\widetilde{\mathcal{M}}_{L\mu}^{(1)}=\widetilde{\mathcal{M}}_{L\mu,-L}^{(1)}+\widetilde{\mathcal{M}}_{L\mu,L+1}^{(1)}, \tag{3.21}$$

with

$$\widetilde{\mathcal{M}}_{L\mu,\kappa}^{(1)}=\left(\frac{\mu_0}{4\pi}\right)^{-1}\frac{\mathrm{sgn}(\kappa)(\kappa-1)^2}{(L+1)^2(2L+1)^2}R_{\kappa}^{(L,L)}(Q^{(0)},P^{(0)};Q^{(0)},P^{(0)})\big[\kappa\mathcal{D}_{L\mu}^{(1)}+\sqrt{L(L+1)}\{\boldsymbol{\nu}\otimes\mathbf{D}_L^{(1)}\}_{L\mu}\big]\quad(\kappa=-L,L+1), \tag{3.22}$$

where

$$\{\boldsymbol{\nu}\otimes\mathbf{D}_L^{(1)}\}_{\lambda\mu}=\sum_{m=-1}^{1}\sum_{M=-L}^{M}\langle 1m;LM|\lambda\mu\rangle\nu_m\mathcal{D}_{LM}^{(1)} \tag{3.23}$$

($\langle j_1m_1;j_2m_2|j_3m_3\rangle$ stands for a Clebsch-Gordan coefficient). From Eqs. (3.15) and (3.20)–(3.22), with the use of the property

$$\{\boldsymbol{\nu}\otimes\mathbf{D}_L^{(1)}\}_{L,-\mu}^{*}=(-)^{\mu+1}\{\boldsymbol{\nu}\otimes\mathbf{D}_L^{(1)}\}_{L\mu} \tag{3.24}$$

of the irreducible spherical tensor product $\{\boldsymbol{\nu}\otimes\mathbf{D}_L^{(1)}\}_L$, we conclude that components of the first-order induced moments are

$$\mathcal{M}_{\lambda\mu}^{(1)}=\mathcal{M}_{\lambda\mu}^{(1)}\delta_{\lambda L}, \tag{3.25}$$

with

$$\mathcal{M}_{L\mu}^{(1)}=\mathcal{M}_{L\mu,-L}^{(1)}+\mathcal{M}_{L\mu,L+1}^{(1)}, \tag{3.26}$$

where

$$\mathcal{M}_{L\mu,\kappa}^{(1)}=\left(\frac{\mu_0}{4\pi}\right)^{-1}\frac{2L|\kappa-1|}{(L+1)(2L+1)^2}\times R_{\kappa}^{(L,L)}(Q^{(0)},P^{(0)};Q^{(0)},P^{(0)})\mathcal{D}_{L\mu}^{(1)}\quad(\kappa=-L,L+1). \tag{3.27}$$

We thus see that, to the first order of the perturbation theory, the 2^L-pole magnetic field induces in the atomic ground state a single magnetic moment of the same multipolarity as that of the perturbing field. Hence, for the total (permanent plus induced) magnetic moments one has

$$\mathbf{M}_\lambda\simeq\mathbf{M}_\lambda^{(0)}\delta_{\lambda1}+\mathbf{M}_\lambda^{(1)}\delta_{\lambda L}. \tag{3.28}$$

B. Atomic multipole magnetizabilities

The 2^L-pole magnetizability (magnetic susceptibility) $\chi_{\mathrm{M}L\to\mathrm{M}L}$ is defined through the relation[2]

$$\mathbf{M}_L^{(1)}=\left(\frac{\mu_0}{4\pi}\right)^{-1}\chi_{\mathrm{M}L\to\mathrm{M}L}\mathbf{D}_L^{(1)}. \tag{3.29}$$

We have separated out the SI factor $(\mu_0/4\pi)^{-1}$ with the intention the physical dimension of $\chi_{\mathrm{M}L\to\mathrm{M}L}$ is $(\text{length})^{2L+1}$. Henceforth, we shall adapt to the most popular notational convention and abbreviate $\chi_{\mathrm{M}L\to\mathrm{M}L}$ to χ_L.

By Eqs. (3.26), (3.27), and (3.29), we see that χ_L may be written in the form

$$\chi_L=\chi_{L,-L}+\chi_{L,L+1}, \tag{3.30}$$

with the constituents of the right-hand side defined as

$$\chi_{L,\kappa}=\frac{2L|\kappa-1|}{(L+1)(2L+1)^2}R_{\kappa}^{(L,L)}(Q^{(0)},P^{(0)};Q^{(0)},P^{(0)})\quad(\kappa=-L,L+1). \tag{3.31}$$

Exploiting Eqs. (3.19) and (2.46), it is found that the component parts $\chi_{L,\kappa}$ of the magnetizability are

$$\chi_{L,\kappa}=\frac{2L|\kappa-1|}{(L+1)(2L+1)^2}\sum_{n_r=-\infty}^{\infty}\frac{1}{\mu_{n_r\kappa}^{(0)}-1}\int_0^{\infty}dr\,r^L\times\big[Q^{(0)}(r)S_{n_r\kappa}^{(0)}(r)+P^{(0)}(r)T_{n_r\kappa}^{(0)}(r)\big]\int_0^{\infty}dr'\,r'^L\times\big[\mu_{n_r\kappa}^{(0)}Q^{(0)}(r')S_{n_r\kappa}^{(0)}(r')+P^{(0)}(r')T_{n_r\kappa}^{(0)}(r')\big]\quad(\kappa=-L,L+1;\ \kappa\neq-1). \tag{3.32}$$

[2]It will be shown in Appendix B that the magnetizability χ_L may be *equivalently* defined with the aid of the formula

$$E^{(2)}=-\frac{1}{2}\left(\frac{\mu_0}{4\pi}\right)^{-1}\chi_L\mathbf{D}_L^{(1)}\cdot\mathbf{D}_L^{(1)},$$

where $E^{(2)}$ is the second-order magnetic-field-induced shift in the energy of the atomic ground state. The reader should be warned that the magnetizability defined in Refs. [18,20,24] is $-(L+1)/2L$ times the one we use.

An exception occurs for $\chi_{1,-1}$, which, by virtue of Eqs. (3.19), (2.47), (2.48), and (2.51), is given by

$$\chi_{1,-1} = \frac{2}{9} \sum_{\substack{n_r=-\infty \\ (n_r \neq 0)}}^{\infty} \frac{1}{\mu^{(0)}_{n_r,-1} - 1} \int_0^\infty dr\, r\big[Q^{(0)}(r)S^{(0)}_{n_r,-1}(r) + P^{(0)}(r)T^{(0)}_{n_r,-1}(r)\big]$$
$$\times \int_0^\infty dr'\, r'\big[\mu^{(0)}_{n_r,-1} Q^{(0)}(r')S^{(0)}_{n_r,-1}(r') + P^{(0)}(r')T^{(0)}_{n_r,-1}(r')\big] - \frac{8}{9}\gamma_1 \frac{a_0}{Z^2}\left[\int_0^\infty dr\, r P^{(0)}(r)Q^{(0)}(r)\right]^2. \tag{3.33}$$

Radial integrals, which appear in Eqs. (3.32) and (3.33), and involve the Sturmians in their integrands, may be evaluated by employing Eqs. (2.16), (2.49), and (2.52), together with the known integration formula [25, Eq. (7.414.11)]

$$\int_0^\infty dx\, x^\gamma e^{-x} L_n^{(\alpha)}(x) = \frac{\Gamma(\gamma+1)\Gamma(n+\alpha-\gamma)}{n!\Gamma(\alpha-\gamma)} \quad (\mathrm{Re}\,\gamma > -1). \tag{3.34}$$

The results are

$$\int_0^\infty dr\, r^L\big[Q^{(0)}(r)S^{(0)}_{n_r\kappa}(r) + P^{(0)}(r)T^{(0)}_{n_r\kappa}(r)\big] = -\alpha Z\left(\frac{a_0}{2Z}\right)^{L+1} \frac{\sqrt{2}(N_{n_r\kappa}-\kappa)}{\sqrt{a_0|n_r|!N_{n_r\kappa}(N_{n_r\kappa}-\kappa)\Gamma(2\gamma_1+1)\Gamma(|n_r|+2\gamma_\kappa+1)}}$$
$$\times \frac{\Gamma(\gamma_\kappa+\gamma_1+L+1)\Gamma(|n_r|+\gamma_\kappa-\gamma_1-L)}{\Gamma(\gamma_\kappa-\gamma_1-L)} \tag{3.35}$$

and

$$\int_0^\infty dr\, r^L\big[\mu^{(0)}_{n_r\kappa} Q^{(0)}(r)S^{(0)}_{n_r\kappa}(r) + P^{(0)}(r)T^{(0)}_{n_r\kappa}(r)\big]$$
$$= \alpha Z\left(\frac{a_0}{2Z}\right)^{L+1} \frac{\big(\mu^{(0)}_{n_r\kappa}-1\big)(N_{n_r\kappa}-\kappa)}{\sqrt{2a_0|n_r|!N_{n_r\kappa}(N_{n_r\kappa}-\kappa)\Gamma(2\gamma_1+1)\Gamma(|n_r|+2\gamma_\kappa+1)}}$$
$$\times \frac{\Gamma(\gamma_\kappa+\gamma_1+L+1)\Gamma(|n_r|+\gamma_\kappa-\gamma_1-L-1)}{\Gamma(\gamma_\kappa-\gamma_1-L)}\left[\kappa-1+\frac{(L+1)(N_{n_r\kappa}+1)}{|n_r|+\gamma_\kappa-\gamma_1}\right] \tag{3.36}$$

[we emphasize that Eqs. (3.35) and (3.36) remain valid also in the case of $L=1$ and $\kappa=-1$].

At this moment, we have in our hands all necessary ingredients to complete calculations of $\chi_{L,\kappa}$, and then χ_L. Plugging Eqs. (2.52), (3.35), and (3.36) into Eqs. (3.32) and (3.33), and then manipulating with the resulting infinite series over n_r just as we did in Ref. [10, Sec. III B], one obtains the sought final expressions for the dipole

$$\chi_1 = -\frac{\alpha^2 a_0^3}{Z^2}\frac{(\gamma_1+1)(4\gamma_1^2-1)}{18}\left\{1+\frac{(\gamma_2+\gamma_1)\Gamma^2(\gamma_2+\gamma_1+2)}{6(2\gamma_1-1)\Gamma(2\gamma_1+3)\Gamma(2\gamma_2+1)}\,{}_3F_2\!\left(\begin{matrix}\gamma_2-\gamma_1-1,\,\gamma_2-\gamma_1-1,\,\gamma_2-\gamma_1\\ \gamma_2-\gamma_1+1,\,2\gamma_2+1\end{matrix};1\right)\right\} \tag{3.37}$$

and higher-order multipole

$$\chi_L = \frac{\alpha^2 a_0^{2L+1}}{Z^{2L}}\frac{L}{2^{2L}(L+1)(2L+1)^2\Gamma(2\gamma_1+1)}\left\{\frac{(L+1)^2\Gamma^2(\gamma_L+\gamma_1+L+1)}{(\gamma_L-\gamma_1)\Gamma(2\gamma_L+1)}\,{}_3F_2\!\left(\begin{matrix}\gamma_L-\gamma_1-L,\,\gamma_L-\gamma_1-L,\,\gamma_L-\gamma_1\\ \gamma_L-\gamma_1+1,\,2\gamma_L+1\end{matrix};1\right)\right.$$
$$\left.-\frac{L^2\Gamma^2(\gamma_{L+1}+\gamma_1+L+1)}{(\gamma_{L+1}-\gamma_1)\Gamma(2\gamma_{L+1}+1)}\,{}_3F_2\!\left(\begin{matrix}\gamma_{L+1}-\gamma_1-L,\,\gamma_{L+1}-\gamma_1-L,\,\gamma_{L+1}-\gamma_1\\ \gamma_{L+1}-\gamma_1+1,\,2\gamma_{L+1}+1\end{matrix};1\right)\right\} \quad (L \geqslant 2) \tag{3.38}$$

magnetizabilities of the Dirac one-electron atom in the ground state, expressed in terms of the generalized hypergeometric functions ${}_3F_2$ of the unit arguments.

The result for the dipole magnetizability displayed in Eq. (3.37) is identical to those presented in Refs. [3,26], and also to those which may be inferred from Refs. [12,18,24]. The reader should be warned that corresponding formulas displayed in Refs. [20,27,28] contain several more or less obvious misprints. As regards higher-order magnetizabilities χ_L with $L \geqslant 2$, the only other pertinent result available in the literature seems to be the one provided in Ref. [18] and reproduced, with some differences, in Ref. [20]. It involves four different ${}_3F_2(1)$ functions, thus being much more complicated than our one in Eq. (3.38), as the latter incorporates only two functions of such kind.

For benchmark purposes, in Table I we provide highly accurate numerical data for the dipole ($L=1$), quadrupole ($L=2$), octupole ($L=3$), and hexadecapole ($L=4$) magnetizabilities for hydrogenic atoms with $Z=1$ and $Z=137$. The numbers have been obtained by coding Eqs. (3.37) and (3.38) in MATHEMATICA. The value of the inverse of the fine-structure constant used has been $\alpha^{-1} = 137.035\,999\,139$ (from CODATA 2014 [29]). All digits displayed are accurate except for the last ones in significands, which are affected by a natural truncation-and-round-off process. It is worthwhile to add that data for $Z=137$ have been obtained

TABLE I. Numerically exact (up to natural truncation-and-round-off errors in the last decimal place) values of the multipole magnetizabilities χ_L with $1 \leqslant L \leqslant 4$ for the ground states of the hydrogen atom ($Z = 1$) and for the hydrogenic ion with $Z = 137$, both with point-charge nuclei, computed from Eq. (3.37) for $L = 1$ and from Eq. (3.38) for $L \geqslant 2$. The value of the inverse of the fine-structure constant used in calculations has been $\alpha^{-1} = 137.035\,999\,139$ (from CODATA 2014).

L	χ_L (units of a_0^{2L+1})	
	$Z = 1$	$Z = 137$
1	$-2.662\,378\,678\,204\,431\,742\,882\,334\times10^{-5}$	$1.147\,344\,605\,832\,761\,686\,544\,069\times10^{-10}$
2	$1.996\,801\,200\,524\,924\,682\,701\,696\times10^{-4}$	$2.558\,468\,317\,313\,541\,963\,409\,678\times10^{-14}$
3	$1.198\,068\,405\,871\,657\,083\,307\,805\times10^{-3}$	$5.280\,642\,300\,945\,502\,538\,135\,788\times10^{-18}$
4	$1.537\,506\,713\,555\,372\,629\,652\,922\times10^{-2}$	$2.459\,574\,506\,149\,252\,615\,931\,133\times10^{-21}$

with the same ease and accuracy as those for $Z = 1$, which is usually not the case in purely numerical approaches based on use of finite differences, Lagrange meshes, or splines.

Numerical values of the lowest-order magnetizabilities with $1 \leqslant L \leqslant 4$ for selected hydrogenic ions in the ground state are presented in Table II. In contrast to the entries of Table I, now the numbers are given in the format which informs how they are influenced by the declared statistical uncertainty (equal to 31) in the last two digits of the CODATA 2014 value of α^{-1}.

For some applications, it may suffice to know approximate expressions for the magnetizabilities valid to the second order in αZ. Such expressions may be derived proceeding analogously as in Ref. [10, Sec. III B], and this leads to the approximations

$$\chi_1 \simeq -\frac{\alpha^2 a_0^3}{Z^2}\frac{1}{2}\left[1 - \frac{4}{3}(\alpha Z)^2\right] \tag{3.39}$$

and

$$\chi_L \simeq \frac{\alpha^2 a_0^{2L+1}}{Z^{2L}}\frac{(3L-1)(2L)!}{2^{2L+1}(L-1)}\Bigg\{1 - (\alpha Z)^2\Bigg[\psi(2L) - \psi(3) + \frac{24L^4 + 15L^3 - L^2 + L + 1}{2L^2(L+1)(2L+1)(3L-1)}\Bigg]\Bigg\} \quad (L \geqslant 2), \tag{3.40}$$

where

$$\psi(z) = \frac{1}{\Gamma(z)}\frac{d\Gamma(z)}{dz} \tag{3.41}$$

is the digamma function. The expressions for quasirelativistic approximations to χ_L with $1 \leqslant L \leqslant 4$, extracted from Eqs. (3.39) and (3.40), are collected in Table III. The result for $L = 1$ fully agrees with those provided in Refs. [26,30] (cf. also Refs. [20,24,27,28]). The value 65/48 for the numerical factor multiplying $(\alpha Z)^2$, given in Ref. [18], is evidently in error and should be replaced by 4/3 (= 64/48). In the quadrupole ($L = 2$) case, Refs. [18,20,24] give the value 167/200 for the numerical factor multiplying $(\alpha Z)^2$, which is in disagreement with our value 703/600. We believe our result is a correct one.

The factors in front of the square bracket on the right-hand side of Eq. (3.39) and in front of the curly brace on the right-hand side of Eq. (3.40) give nonrelativistic multipole magnetizabilities χ_L^{NR} for hydrogenic ions in the ground state. The result for the dipole magnetizability,

$$\chi_1^{\mathrm{NR}} = -\frac{1}{2}\frac{\alpha^2 a_0^3}{Z^2}, \tag{3.42}$$

coincides with the one well known from the literature (see, e.g., Ref. [28, Eq. (2.4.32)]). The formula

$$\chi_L^{\mathrm{NR}} = \frac{\alpha^2 a_0^{2L+1}}{Z^{2L}}\frac{(3L-1)(2L)!}{2^{2L+1}(L-1)} \quad (L \geqslant 2) \tag{3.43}$$

for higher-order magnetizabilities is in agreement with the finding of Manakov *et al.* [18,20,24] (observe, however, that an expression given in Ref. [18] may be simplified considerably), after differences in definitions used are taken into account (cf. footnote 2 of the present work). Somewhat surprisingly, we

TABLE II. The static multipole magnetizabilities χ_L with $1 \leqslant L \leqslant 4$ for selected hydrogenic ions in the ground state, computed from the analytical formulas in Eqs. (3.37) and (3.38). The number in parentheses following each significand is an uncertainty in its last two digits, and stems from the one-standard-deviation uncertainty (equal to 31) in the last two digits of the value of the inverse of the fine-structure constant $\alpha^{-1} = 137.035\,999\,139$ (from CODATA 2014) used in calculations.

Z	χ_1 (units of a_0^3)	χ_2 (units of a_0^5)	χ_3 (units of a_0^7)	χ_4 (units of a_0^9)
1	$-2.662\,378\,678\,2\,(12)\times10^{-5}$	$1.996\,801\,200\,52\,(91)\times10^{-4}$	$1.198\,068\,405\,87\,(54)\times10^{-3}$	$1.537\,506\,713\,56\,(70)\times10^{-2}$
2	$-6.654\,528\,896\,0\,(30)\times10^{-6}$	$1.247\,767\,150\,68\,(57)\times10^{-5}$	$1.871\,573\,772\,48\,(85)\times10^{-5}$	$6.004\,407\,447\,2\,(27)\times10^{-5}$
5	$-1.063\,136\,977\,70\,(48)\times10^{-6}$	$3.190\,098\,991\,1\,(15)\times10^{-7}$	$7.654\,269\,671\,4\,(35)\times10^{-8}$	$3.928\,271\,052\,8\,(18)\times10^{-8}$
10	$-2.643\,677\,394\,3\,(12)\times10^{-7}$	$1.984\,481\,176\,33\,(89)\times10^{-8}$	$1.189\,463\,455\,15\,(54)\times10^{-9}$	$1.525\,046\,102\,84\,(69)\times10^{-10}$
20	$-6.467\,948\,998\,0\,(29)\times10^{-8}$	$1.217\,077\,812\,35\,(54)\times10^{-9}$	$1.818\,075\,902\,10\,(80)\times10^{-11}$	$5.811\,030\,078\,2\,(26)\times10^{-13}$
40	$-1.477\,390\,017\,82\,(59)\times10^{-8}$	$7.036\,528\,266\,0\,(28)\times10^{-11}$	$2.594\,464\,562\,8\,(10)\times10^{-13}$	$2.049\,184\,462\,11\,(80)\times10^{-15}$
60	$-5.559\,035\,106\,2\,(17)\times10^{-9}$	$1.209\,460\,538\,56\,(41)\times10^{-11}$	$1.937\,732\,430\,73\,(61)\times10^{-14}$	$6.664\,062\,860\,1\,(20)\times10^{-17}$
80	$-2.367\,686\,026\,55\,(31)\times10^{-9}$	$3.075\,158\,743\,53\,(65)\times10^{-12}$	$2.676\,175\,877\,74\,(46)\times10^{-15}$	$5.015\,954\,916\,67\,(68)\times10^{-18}$
100	$-9.318\,033\,458\,0\,(28)\times10^{-10}$	$8.966\,282\,348\,22\,(28)\times10^{-13}$	$4.736\,237\,750\,50\,(50)\times10^{-16}$	$5.417\,345\,278\,73\,(93)\times10^{-19}$
120	$-2.044\,067\,541\,7\,(51)\times10^{-10}$	$2.409\,493\,920\,8\,(16)\times10^{-13}$	$8.100\,744\,853\,2\,(67)\times10^{-17}$	$5.955\,659\,278\,5\,(57)\times10^{-20}$
137	$+1.147\,344\,605\,8\,(46)\times10^{-10}$	$2.558\,468\,32\,(12)\times10^{-14}$	$5.280\,642\,30\,(27)\times10^{-18}$	$2.459\,574\,51\,(14)\times10^{-21}$

TABLE III. Quasirelativistic approximations for the static multipole magnetizabilities χ_L with $1 \leqslant L \leqslant 4$ for the Dirac one-electron atom in the ground state. The expressions for which $L \geqslant 2$ have been derived from Eq. (3.40).

L	χ_L
1	$-\frac{\alpha^2 a_0^3}{Z^2}\,\frac{1}{2}[1-\frac{4}{3}(\alpha Z)^2]$
2	$\frac{\alpha^2 a_0^5}{Z^4}\,\frac{15}{4}[1-\frac{703}{600}(\alpha Z)^2]$
3	$\frac{\alpha^2 a_0^7}{Z^6}\,\frac{45}{2}[1-\frac{3439}{2520}(\alpha Z)^2]$
4	$\frac{\alpha^2 a_0^9}{Z^8}\,\frac{1155}{4}[1-\frac{170827}{110880}(\alpha Z)^2]$

have been unable to track down in the literature any other publication with an independently derived expression for χ_L^{NR} with $L \geqslant 2$.

IV. ELECTRIC MULTIPOLE MOMENTS OF THE ATOM IN THE MULTIPOLE MAGNETIC FIELD AND ATOMIC M$L \to$ E$(L \mp 1)$ MULTIPOLE CROSS-SUSCEPTIBILITIES

A. Decomposition of the atomic electric multipole moments into the permanent and the first-order magnetic-field-induced components

The far-field static electric 2^λ-pole moment of the atomic electronic cloud in the stationary state characterized by the wave function $\Psi(\boldsymbol{r})$ is defined as [10, Appendix B]

$$\mathcal{Q}_{\lambda\mu} = \sqrt{\frac{4\pi}{2\lambda+1}} \int_{\mathbb{R}^3} d^3\boldsymbol{r}\, r^\lambda Y_{\lambda\mu}(\boldsymbol{n}_r)\rho(\boldsymbol{r}), \tag{4.1}$$

where

$$\rho(\boldsymbol{r}) = \frac{-e\Psi^\dagger(\boldsymbol{r})\Psi(\boldsymbol{r})}{\int_{\mathbb{R}^3} d^3\boldsymbol{r}'\, \Psi^\dagger(\boldsymbol{r}')\Psi(\boldsymbol{r}')} \tag{4.2}$$

is the electronic charge density. In the weak external perturbing field, under the assumptions displayed in Eqs. (2.18) and (2.21), the density in Eq. (4.2) may be approximated as

$$\rho(\boldsymbol{r}) \simeq \rho^{(0)}(\boldsymbol{r}) + \rho^{(1)}(\boldsymbol{r}), \tag{4.3}$$

with

$$\rho^{(0)}(\boldsymbol{r}) = -e\Psi^{(0)\dagger}(\boldsymbol{r})\Psi^{(0)}(\boldsymbol{r}) \tag{4.4}$$

and

$$\rho^{(1)}(\boldsymbol{r}) = -2e\,\mathrm{Re}[\Psi^{(0)\dagger}(\boldsymbol{r})\Psi^{(1)}(\boldsymbol{r})]. \tag{4.5}$$

This implies the approximation

$$\mathcal{Q}_{\lambda\mu} \simeq \mathcal{Q}_{\lambda\mu}^{(0)} + \mathcal{Q}_{\lambda\mu}^{(1)}, \tag{4.6}$$

with

$$\mathcal{Q}_{\lambda\mu}^{(0)} = \sqrt{\frac{4\pi}{2\lambda+1}} \int_{\mathbb{R}^3} d^3\boldsymbol{r}\, r^\lambda Y_{\lambda\mu}(\boldsymbol{n}_r)\rho^{(0)}(\boldsymbol{r}) \tag{4.7}$$

and

$$\mathcal{Q}_{\lambda\mu}^{(1)} = \sqrt{\frac{4\pi}{2\lambda+1}} \int_{\mathbb{R}^3} d^3\boldsymbol{r}\, r^\lambda Y_{\lambda\mu}(\boldsymbol{n}_r)\rho^{(1)}(\boldsymbol{r}). \tag{4.8}$$

It has been shown in Ref. [10] that the only nonzero permanent electric multipole moment of the electronic cloud in the ground state of the isolated atom is the monopole one:

$$\mathcal{Q}_{\lambda\mu}^{(0)} = \mathcal{Q}_{\lambda\mu}^{(0)}\delta_{\lambda 0}\delta_{\mu 0}, \quad \mathcal{Q}_{00}^{(0)} = -e. \tag{4.9}$$

As concerns the components $\mathcal{Q}_{\lambda\mu}^{(1)}$ of the induced moments, they may be evaluated in a manner very much similar to that which has led us from Eq. (3.8) to Eq. (3.27), and therefore we omit details. At the end, one finds that

$$\mathcal{Q}_{\lambda\mu}^{(1)} = \mathcal{Q}_{\lambda\mu}^{(1)}[\delta_{\lambda,L-1}(1-\delta_{L1}) + \delta_{\lambda,L+1}], \tag{4.10}$$

with

$$\begin{aligned}\mathcal{Q}_{\lambda\mu}^{(1)} = {}& \left(\frac{\mu_0}{4\pi}\right)^{-1} c^{-1} \frac{2L(\lambda-L)}{(2\lambda+1)(2L+1)} \\ & \times R_{-\kappa_{\lambda L}}^{(\lambda,L)}(P^{(0)},Q^{(0)};Q^{(0)},P^{(0)}) \frac{\{\boldsymbol{\nu}\otimes\mathbf{D}_L^{(1)}\}_{\lambda\mu}}{\langle 10;L0|\lambda 0\rangle} \\ & (\lambda = L\mp 1,\ \lambda\neq 0),\end{aligned} \tag{4.11}$$

where

$$\langle 10;L0|\lambda 0\rangle = (\lambda-L)\sqrt{\frac{\lambda+L+1}{2(2L+1)}} \quad (\lambda = L\mp 1), \tag{4.12}$$

while

$$\kappa_{\lambda L} = -\frac{1}{2}(\lambda-L)(\lambda+L+1) = \begin{cases} L & \text{for } \lambda = L-1 \\ -L-1 & \text{for } \lambda = L+1. \end{cases} \tag{4.13}$$

Thus, the 2^L-pole magnetic field induces in the ground state of the Dirac one-electron atom electric moments of multipolarities 2^{L+1} and 2^{L-1}, provided that $L \neq 1$. In the latter case, when the perturbing magnetic field is the dipole one, only a quadrupole electric moment is induced. [Mathematically, vanishing of $\mathcal{Q}_{00}^{(1)}$ is a consequence of the orthogonality of $\Psi^{(1)}(\boldsymbol{r})$ to $\Psi^{(0)}(\boldsymbol{r})$; physically, this reflects the obvious fact that the perturbing field cannot induce a net electric charge in the atom.] For the total (permanent plus induced) electric moment of the electronic cloud, one thus has

$$\mathbf{Q}_\lambda \simeq \mathbf{Q}_\lambda^{(0)}\delta_{\lambda 0} + \mathbf{Q}_\lambda^{(1)}[\delta_{\lambda,L-1}(1-\delta_{L1}) + \delta_{\lambda,L+1}]. \tag{4.14}$$

B. Atomic multipole M$L \to$ E$(L \mp 1)$ cross-susceptibilities

We define a magnetic-to-electric cross-susceptibility $\chi_{\mathrm{M}L\to\mathrm{E}\lambda}$ through the formula

$$\mathbf{Q}_\lambda^{(1)} = \left(\frac{\mu_0}{4\pi}\right)^{-1} c^{-1} \chi_{\mathrm{M}L\to\mathrm{E}\lambda} \frac{\{\boldsymbol{\nu}\otimes\mathbf{D}_L^{(1)}\}_\lambda}{\langle 10;L0|\lambda 0\rangle} \quad (\lambda = L\mp 1,\ \lambda\neq 0). \tag{4.15}$$

It is evident that the physical dimension of $\chi_{\mathrm{M}L\to\mathrm{E}\lambda}$ is $(\text{length})^{\lambda+L+1}$. Comparison of Eqs. (4.15) and (4.11) yields the cross-susceptibility in question in the form

$$\chi_{\mathrm{M}L\to\mathrm{E}\lambda} = \frac{2L(\lambda-L)}{(2\lambda+1)(2L+1)} R_{-\kappa_{\lambda L}}^{(\lambda,L)}(P^{(0)},Q^{(0)};Q^{(0)},P^{(0)}) \quad (\lambda = L\mp 1,\ \lambda\neq 0). \tag{4.16}$$

In Ref. [10], we have defined and investigated a counterpart quantity $\alpha_{\mathrm{E}L\to\mathrm{M}\lambda}$—the electric-to-magnetic cross-susceptibility—which characterizes a 2^λ-pole magnetic moment induced in the atom by an external 2^L-pole electric field.

In particular, we have shown that $\alpha_{\mathrm{E}L\to\mathrm{M}\lambda}$ can be written as

$$\alpha_{\mathrm{E}L\to\mathrm{M}\lambda} = -\frac{2\lambda(\lambda-L)}{(2\lambda+1)(2L+1)} R^{(\lambda,L)}_{\kappa_{\lambda L}}(Q^{(0)},P^{(0)};P^{(0)},Q^{(0)}) \quad (\lambda = L\mp 1,\ \lambda\neq 0). \tag{4.17}$$

Now, we shall make two observations. First, it follows from the definition (3.19) and the identity

$$\bar{\mathsf{G}}^{(0)}_{\kappa}(r,r') = \bar{\mathsf{G}}^{(0)\mathrm{T}}_{\kappa}(r',r) \tag{4.18}$$

(here T denotes the matrix transpose) obeyed by the radial generalized Green function that the double radial integral $R^{(L_1,L_2)}_{\kappa}(F_a,F_b;F_c,F_d)$ possesses the symmetry property

$$R^{(L_1,L_2)}_{\kappa}(F_a,F_b;F_c,F_d) = R^{(L_2,L_1)}_{\kappa}(F_c,F_d;F_a,F_b). \tag{4.19}$$

Second, from Eq. (4.13) one easily infers that

$$-\kappa_{\lambda L} = \kappa_{L\lambda}. \tag{4.20}$$

On combining Eqs. (4.16), (4.17), (4.19), and (4.20), we arrive at the relationship

$$\chi_{\mathrm{M}L\to\mathrm{E}(L\mp1)} = \alpha_{\mathrm{E}(L\mp1)\to\mathrm{M}L}, \tag{4.21}$$

with $L\geqslant 2$ ($L\geqslant 1$) in the upper (lower) sign case. The identity (4.21) allows us to deduce exact and approximate expressions for $\chi_{\mathrm{M}L\to\mathrm{E}(L\mp1)}$ from those given in Ref. [10, Sec. IV.B] for $\alpha_{\mathrm{E}L\to\mathrm{M}(L\mp1)}$, after the simultaneous replacements $L\to\lambda(=L\mp1)$ and $\lambda\to L$ are made in the latter. Proceeding in that way, we arrive at the general formula

$$\begin{aligned}\chi_{\mathrm{M}L\to\mathrm{E}\lambda} = {}& \frac{\alpha a_0^{\lambda+L+1}}{Z^{\lambda+L+1}} \frac{L(L-\lambda)\Gamma(2\gamma_1+\lambda+L+2)}{2^{\lambda+L}(\kappa_{\lambda L}-1)(2\lambda+1)(2L+1)\Gamma(2\gamma_1+1)}\\ &\times\left\{1+\frac{(L+1)[\gamma_1(\kappa_{\lambda L}-1)-\lambda-1]\Gamma(\gamma_{\kappa_{\lambda L}}+\gamma_1+\lambda+1)\Gamma(\gamma_{\kappa_{\lambda L}}+\gamma_1+L+1)}{(\gamma_{\kappa_{\lambda L}}-\gamma_1+1)\Gamma(2\gamma_1+\lambda+L+2)\Gamma(2\gamma_{\kappa_{\lambda L}}+1)}\right.\\ &\left.\times\,{}_3F_2\left(\begin{matrix}\gamma_{\kappa_{\lambda L}}-\gamma_1-\lambda,\ \gamma_{\kappa_{\lambda L}}-\gamma_1-L,\ \gamma_{\kappa_{\lambda L}}-\gamma_1+1\\ \gamma_{\kappa_{\lambda L}}-\gamma_1+2,\ 2\gamma_{\kappa_{\lambda L}}+1\end{matrix};1\right)\right\} \quad (\lambda=L\mp1,\ \lambda\neq0),\end{aligned} \tag{4.22}$$

which particularizes to

$$\begin{aligned}\chi_{\mathrm{M}L\to\mathrm{E}(L-1)} = {}& \frac{\alpha a_0^{2L}}{Z^{2L}} \frac{L\Gamma(2\gamma_1+2L+1)}{2^{2L-1}(L-1)(4L^2-1)\Gamma(2\gamma_1+1)}\\ &\times\left\{1+\frac{(L+1)[\gamma_1(L-1)-L]\Gamma(\gamma_L+\gamma_1+L)\Gamma(\gamma_L+\gamma_1+L+1)}{(\gamma_L-\gamma_1+1)\Gamma(2\gamma_1+2L+1)\Gamma(2\gamma_L+1)}\right.\\ &\left.\times\,{}_3F_2\left(\begin{matrix}\gamma_L-\gamma_1-L,\ \gamma_L-\gamma_1-L+1,\ \gamma_L-\gamma_1+1\\ \gamma_L-\gamma_1+2,\ 2\gamma_L+1\end{matrix};1\right)\right\} \quad (L\geqslant 2)\end{aligned} \tag{4.23}$$

and

$$\begin{aligned}\chi_{\mathrm{M}L\to\mathrm{E}(L+1)} = {}& \frac{\alpha a_0^{2L+2}}{Z^{2L+2}} \frac{L\Gamma(2\gamma_1+2L+3)}{2^{2L+1}(L+2)(2L+1)(2L+3)\Gamma(2\gamma_1+1)}\\ &\times\left\{1-\frac{(L+1)(L+2)(\gamma_1+1)\Gamma(\gamma_{L+1}+\gamma_1+L+1)\Gamma(\gamma_{L+1}+\gamma_1+L+2)}{(\gamma_{L+1}-\gamma_1+1)\Gamma(2\gamma_1+2L+3)\Gamma(2\gamma_{L+1}+1)}\right.\\ &\left.\times\,{}_3F_2\left(\begin{matrix}\gamma_{L+1}-\gamma_1-L-1,\ \gamma_{L+1}-\gamma_1-L,\ \gamma_{L+1}-\gamma_1+1\\ \gamma_{L+1}-\gamma_1+2,\ 2\gamma_{L+1}+1\end{matrix};1\right)\right\}.\end{aligned} \tag{4.24}$$

In the dipole ($L=1$) case, Eq. (4.24) becomes

$$\chi_{\mathrm{M}1\to\mathrm{E}2} = \frac{\alpha a_0^4}{Z^4}\frac{\Gamma(2\gamma_1+5)}{360\Gamma(2\gamma_1+1)}\left\{1-\frac{6(\gamma_1+1)\Gamma(\gamma_2+\gamma_1+2)\Gamma(\gamma_2+\gamma_1+3)}{(\gamma_2-\gamma_1+1)\Gamma(2\gamma_1+5)\Gamma(2\gamma_2+1)}\,{}_3F_2\left(\begin{matrix}\gamma_2-\gamma_1-2,\ \gamma_2-\gamma_1-1,\ \gamma_2-\gamma_1+1\\ \gamma_2-\gamma_1+2,\ 2\gamma_2+1\end{matrix};1\right)\right\}. \tag{4.25}$$

This agrees with the result which may be inferred from Ref. [8, Eq. (4.20)], after the latter is transformed with the aid of the identity

$$\begin{aligned}{}_3F_2\left(\begin{matrix}a_1,\ a_2,\ a_3\\ a_3+1,\ b\end{matrix};1\right) = {}& \frac{\Gamma(b)\Gamma(b-a_1-a_2+1)}{(b-a_3-1)\Gamma(b-a_1)\Gamma(b-a_2)} - \frac{(a_1-a_3-1)(a_2-a_3-1)}{(a_3+1)(b-a_3-1)}\,{}_3F_2\left(\begin{matrix}a_1,\ a_2,\ a_3+1\\ a_3+2,\ b\end{matrix};1\right)\\ &[\mathrm{Re}(b-a_1-a_2)>-1].\end{aligned} \tag{4.26}$$

Numerical values for the cross-susceptibilities $\chi_{\mathrm{M}L\to\mathrm{E}(L\mp1)}$ with $1\leqslant L\leqslant 4$, computed for selected hydrogenic ions from Eqs. (4.23) and (4.24), are presented in Tables IV and V.

TABLE IV. The static magnetic-to-electric cross-susceptibilities $\chi_{\mathrm{M}L\to\mathrm{E}(L-1)}$ with $2 \leqslant L \leqslant 4$ for selected hydrogenic ions in the ground state, computed from the analytical formula in Eq. (4.23). The number in parentheses following each significand is an uncertainty in its last two digits, and stems from the one-standard-deviation uncertainty (equal to 31) in the last two digits of the value of the inverse of the fine-structure constant $\alpha^{-1} = 137.035\,999\,139$ (from CODATA 2014) used in calculations.

Z	$\chi_{\mathrm{M2}\to\mathrm{E1}}$ (units of a_0^4)	$\chi_{\mathrm{M3}\to\mathrm{E2}}$ (units of a_0^6)	$\chi_{\mathrm{M4}\to\mathrm{E3}}$ (units of a_0^8)
1	3.283 609 988 21 (74)$\times10^{-2}$	1.641 779 910 28 (37)$\times10^{-1}$	1.915 387 218 71 (44)
2	2.051 883 757 57 (47)$\times10^{-3}$	2.564 697 947 34 (58)$\times10^{-3}$	7.480 014 760 8 (17)$\times10^{-3}$
5	5.246 149 090 0 (12)$\times10^{-5}$	1.048 828 974 42 (24)$\times10^{-5}$	4.893 086 196 1 (11)$\times10^{-6}$
10	3.263 961 669 54 (73)$\times10^{-6}$	1.629 485 276 85 (36)$\times10^{-7}$	1.898 813 208 63 (42)$\times10^{-8}$
20	2.002 912 101 25 (43)$\times10^{-7}$	2.488 285 199 83 (53)$\times10^{-9}$	7.222 989 034 9 (15)$\times10^{-11}$
40	1.160 561 045 67 (21)$\times10^{-8}$	3.536 787 823 83 (59)$\times10^{-11}$	2.529 227 814 95 (40)$\times10^{-13}$
60	2.001 899 182 26 (22)$\times10^{-9}$	2.622 086 172 86 (22)$\times10^{-12}$	8.120 641 172 46 (49)$\times10^{-15}$
80	5.112 923 654 384 (67)$\times10^{-10}$	3.576 878 765 05 (25)$\times10^{-13}$	5.987 127 613 93 (69)$\times10^{-16}$
100	1.497 342 934 87 (38)$\times10^{-10}$	6.199 237 022 9 (23)$\times10^{-14}$	6.253 163 632 3 (28)$\times10^{-17}$
120	4.025 596 828 3 (36)$\times10^{-11}$	1.018 161 258 7 (12)$\times10^{-14}$	6.466 767 859 0 (85)$\times10^{-18}$
137	4.095 281 71 (19)$\times10^{-12}$	5.745 732 04 (32)$\times10^{-16}$	2.193 610 03 (14)$\times10^{-19}$

The quasirelativistic approximations to the expressions displayed in Eqs. (4.23) and (4.24) are

$$\chi_{\mathrm{M}L\to\mathrm{E}(L-1)} \simeq \frac{\alpha a_0^{2L}}{Z^{2L}}\frac{(L+1)(2L)!}{2^{2L}(L-1)}\left\{1-(\alpha Z)^2\left[\psi(2L+2)-\psi(2) - \frac{(L-1)(2L^4+L^3+2L^2+2L+1)}{2L^2(L+1)(2L-1)(2L+1)}\right]\right\} \quad (L \geqslant 2) \tag{4.27}$$

and

$$\chi_{\mathrm{M}L\to\mathrm{E}(L+1)} \simeq \frac{\alpha a_0^{2L+2}}{Z^{2L+2}}(\alpha Z)^2\frac{L^2(2L^3+11L^2+20L+13)(2L)!}{2^{2L+2}(L+1)(L+2)(2L+3)}, \tag{4.28}$$

respectively. Explicit representations deduced from Eqs. (4.27) and (4.28) for $1 \leqslant L \leqslant 4$ are collected in Table VI.

V. NEAR-NUCLEUS MAGNETIC MULTIPOLE MOMENTS OF THE ATOM IN THE MULTIPOLE MAGNETIC FIELD AND MAGNETIC MULTIPOLE NUCLEAR SHIELDING CONSTANTS

Spherical components of the near-field magnetic multipole moment N_λ associated with the current distribution $\boldsymbol{j}(\boldsymbol{r})$ are defined as [10, Appendix B.3]

$$\mathcal{N}_{\lambda\mu} = i\sqrt{\frac{4\pi(\lambda+1)}{\lambda(2\lambda+1)}}\int_{\mathbb{R}^3} d^3\boldsymbol{r}\, r^{-\lambda-1}\boldsymbol{Y}^{\lambda}_{\lambda\mu}(\boldsymbol{n}_r)\cdot\boldsymbol{j}(\boldsymbol{r}). \tag{5.1}$$

For the atomic system under study the current $\boldsymbol{j}(\boldsymbol{r})$ is the one in Eq. (3.2). Use of the approximation (3.3) yields

$$\mathcal{N}_{\lambda\mu} \simeq \mathcal{N}^{(0)}_{\lambda\mu} + \mathcal{N}^{(1)}_{\lambda\mu}, \tag{5.2}$$

with

$$\mathcal{N}^{(0)}_{\lambda\mu} = i\sqrt{\frac{4\pi(\lambda+1)}{\lambda(2\lambda+1)}}\int_{\mathbb{R}^3} d^3\boldsymbol{r}\, r^{-\lambda-1}\boldsymbol{Y}^{\lambda}_{\lambda\mu}(\boldsymbol{n}_r)\cdot\boldsymbol{j}^{(0)}(\boldsymbol{r}) \tag{5.3}$$

TABLE V. The static magnetic-to-electric cross-susceptibilities $\chi_{\mathrm{M}L\to\mathrm{E}(L+1)}$ with $1 \leqslant L \leqslant 4$ for selected hydrogenic ions in the ground state, computed from the analytical formula in Eq. (4.24). The number in parentheses following each significand is an uncertainty in its last two digits, and stems from the one-standard-deviation uncertainty (equal to 31) in the last two digits of the value of the inverse of the fine-structure constant $\alpha^{-1} = 137.035\,999\,139$ (from CODATA 2014) used in calculations.

Z	$\chi_{\mathrm{M1}\to\mathrm{E2}}$ (units of a_0^4)	$\chi_{\mathrm{M2}\to\mathrm{E3}}$ (units of a_0^6)	$\chi_{\mathrm{M3}\to\mathrm{E4}}$ (units of a_0^8)	$\chi_{\mathrm{M4}\to\mathrm{E5}}$ (units of a_0^{10})
1	7.447 801 428 7 (51)$\times10^{-8}$	7.840 878 107 8 (53)$\times10^{-7}$	1.234 923 524 98 (84)$\times10^{-5}$	2.944 977 893 0 (20)$\times10^{-4}$
2	1.861 763 994 3 (13)$\times10^{-8}$	4.899 814 158 6 (34)$\times10^{-8}$	1.929 209 479 8 (13)$\times10^{-7}$	1.150 135 134 26 (78)$\times10^{-6}$
5	2.976 734 913 0 (21)$\times10^{-9}$	1.253 036 091 45 (85)$\times10^{-9}$	7.891 765 327 7 (54)$\times10^{-10}$	7.526 205 826 1 (51)$\times10^{-10}$
10	7.423 191 448 8 (51)$\times10^{-10}$	7.802 108 784 5 (53)$\times10^{-11}$	1.227 360 291 30 (83)$\times10^{-11}$	2.924 158 478 3 (20)$\times10^{-12}$
20	1.837 121 846 2 (13)$\times10^{-10}$	4.803 053 653 1 (32)$\times10^{-12}$	1.882 114 263 5 (13)$\times10^{-13}$	1.117 776 688 30 (74)$\times10^{-14}$
40	4.404 779 739 7 (29)$\times10^{-11}$	2.820 265 342 7 (18)$\times10^{-13}$	2.722 166 133 1 (17)$\times10^{-15}$	3.993 935 630 7 (25)$\times10^{-17}$
60	1.816 173 088 1 (11)$\times10^{-11}$	4.983 382 447 9 (29)$\times10^{-14}$	2.082 589 394 7 (12)$\times10^{-16}$	1.329 890 711 11 (73)$\times10^{-18}$
80	9.069 233 476 7 (50)$\times10^{-12}$	1.323 207 519 24 (64)$\times10^{-14}$	2.987 634 353 8 (14)$\times10^{-17}$	1.039 173 156 16 (42)$\times10^{-19}$
100	4.810 527 179 2 (20)$\times10^{-12}$	4.126 084 143 0 (12)$\times10^{-15}$	5.611 810 738 7 (12)$\times10^{-18}$	1.190 427 803 76 (17)$\times10^{-20}$
120	2.398 905 441 474 (94)$\times10^{-12}$	1.243 760 509 44 (27)$\times10^{-15}$	1.064 754 960 93 (42)$\times10^{-18}$	1.451 110 265 85 (78)$\times10^{-21}$
137	6.535 200 35 (19)$\times10^{-13}$	1.835 801 306 (67)$\times10^{-16}$	9.459 904 27 (40)$\times10^{-20}$	8.182 983 16 (38)$\times10^{-23}$

TABLE VI. Quasirelativistic approximations for the static magnetic-to-electric cross-susceptibilities $\chi_{\mathrm{M}L\to\mathrm{E}(L-1)}$ with $2\leqslant L\leqslant 4$ and $\chi_{\mathrm{M}L\to\mathrm{E}(L+1)}$ with $1\leqslant L\leqslant 4$ for the Dirac one-electron atom in the ground state. The expressions have been derived from Eqs. (4.27) and (4.28).

L	$\chi_{\mathrm{M}L\to\mathrm{E}(L-1)}$	$\chi_{\mathrm{M}L\to\mathrm{E}(L+1)}$
1		$\frac{\alpha a_0^4}{Z^4}\frac{23}{120}(\alpha Z)^2$
2	$\frac{\alpha a_0^4}{Z^4}\frac{9}{2}[1-\frac{409}{360}(\alpha Z)^2]$	$\frac{\alpha a_0^6}{Z^6}\frac{113}{56}(\alpha Z)^2$
3	$\frac{\alpha a_0^6}{Z^6}\frac{45}{2}[1-\frac{1793}{1260}(\alpha Z)^2]$	$\frac{\alpha a_0^8}{Z^8}\frac{1017}{32}(\alpha Z)^2$
4	$\frac{\alpha a_0^8}{Z^8}\frac{525}{2}[1-\frac{3317}{2016}(\alpha Z)^2]$	$\frac{\alpha a_0^{10}}{Z^{10}}\frac{8337}{11}(\alpha Z)^2$

and

$$\mathcal{N}_{\lambda\mu}^{(1)}=i\sqrt{\frac{4\pi(\lambda+1)}{\lambda(2\lambda+1)}}\int_{\mathbb{R}^3}d^3\boldsymbol{r}\,r^{-\lambda-1}\boldsymbol{Y}_{\lambda\mu}^{\lambda}(\boldsymbol{n}_r)\cdot\boldsymbol{j}^{(1)}(\boldsymbol{r}),\quad(5.4)$$

where $\mathcal{N}_{\lambda\mu}^{(0)}$ and $\mathcal{N}_{\lambda\mu}^{(1)}$ are components of the rank-λ tensors $\mathbf{N}_{\lambda}^{(0)}$ and $\mathbf{N}_{\lambda}^{(1)}$, respectively. The unperturbed current $\boldsymbol{j}^{(0)}(\boldsymbol{r})$ and the first-order induced current $\boldsymbol{j}^{(1)}(\boldsymbol{r})$ appearing in the above equations have been defined in Eqs. (3.4) and (3.5), respectively. Carrying out angular integrations in the manner similar to the one in Sec. III, one finds that

$$\mathbf{N}_{\lambda}\simeq\mathbf{N}_{\lambda}^{(0)}\delta_{\lambda1}+\mathbf{N}_{\lambda}^{(1)}\delta_{\lambda L}.\quad(5.5)$$

The only nonvanishing permanent near-nucleus magnetic multipole moment of the atom is the dipole one and is explicitly given by (cf. Ref. [10, Eq. (7.9)])

$$\mathbf{N}_{1}^{(0)}=\frac{8}{3\gamma_1(2\gamma_1-1)}\frac{\mu_{\mathrm{B}}Z^3}{a_0^3}\boldsymbol{\nu}\quad\left(Z<\alpha^{-1}\frac{\sqrt{3}}{2}\right).\quad(5.6)$$

On the other side, the only nonzero induced near-nucleus magnetic multipole moment of the atom is the 2^L-pole one, and is found to be of the form

$$\mathbf{N}_{L}^{(1)}=\left(\frac{\mu_0}{4\pi}\right)^{-1}\sigma_{\mathrm{M}L\to\mathrm{M}L}\mathbf{D}_{L}^{(1)}.\quad(5.7)$$

The coefficient $\sigma_{\mathrm{M}L\to\mathrm{M}L}$ is the 2^L-pole nuclear magnetic shielding constant. For $L=1$ one finds that

$$\sigma_{\mathrm{M1}\to\mathrm{M1}}=-\alpha^2Z\frac{2(4\gamma_1^3+6\gamma_1^2-7\gamma_1-12)}{27\gamma_1(\gamma_1+1)(2\gamma_1-1)}\quad\left(Z<\alpha^{-1}\frac{\sqrt{3}}{2}\right),\quad(5.8)$$

while for $L\geqslant 2$ the corresponding expression is

$$\sigma_{\mathrm{M}L\to\mathrm{M}L}=-\alpha^2Z\frac{2}{(2L+1)^2}\left\{\frac{(L+1)^2}{(\gamma_L-\gamma_1)(\gamma_L+\gamma_1-L)}\,{}_3F_2\left(\begin{matrix}-L,\,1,\,\gamma_L-\gamma_1-L\\ \gamma_L-\gamma_1+1,\,\gamma_L+\gamma_1-L+1\end{matrix};1\right)-\frac{L^2}{(\gamma_{L+1}-\gamma_1)(\gamma_{L+1}+\gamma_1-L)}\right.$$
$$\left.\times\,{}_3F_2\left(\begin{matrix}-L,\,1,\,\gamma_{L+1}-\gamma_1-L\\ \gamma_{L+1}-\gamma_1+1,\,\gamma_{L+1}+\gamma_1-L+1\end{matrix};1\right)\right\}\quad\left(L\geqslant 2;\ Z<\alpha^{-1}\frac{\sqrt{4L^2-1}}{2L}\right).\quad(5.9)$$

It should be observed that both hypergeometric functions which appear in Eq. (5.9) are truncating ones, and consequently not only the dipole shielding constant $\sigma_{\mathrm{M1}\to\mathrm{M1}}$, but also those with $L\geqslant 2$, may be expressed in terms of elementary functions. For the reader's convenience, in Table VII we collect such simple exact expressions for $\sigma_{\mathrm{M}L\to\mathrm{M}L}$ with $1\leqslant L\leqslant 4$.

The formula for the dipole shielding constant $\sigma_{\mathrm{M1}\to\mathrm{M1}}$ displayed in Eq. (5.8) is identical with the one presented in Refs. [7,15]. With some algebra, it may also be shown to coincide with the results given in Refs. [31,32]. The counterpart expression derived in Ref. [19] (cf. also Refs. [20,24]) should be corrected in that in its denominator the factor λ_2 should be replaced by λ_1 (being our γ_1). Our result (5.9) for $\sigma_{\mathrm{M}L\to\mathrm{M}L}$ with $L\geqslant 2$ contains two truncating ${}_3F_2(1)$ functions and is definitely simpler than the one derived in Ref. [19] (cf. also Ref. [20]), where four such functions are involved implicitly.

TABLE VII. Exact analytical expressions for the static magnetic multipole nuclear shielding constants $\sigma_{\mathrm{M}L\to\mathrm{M}L}$ with $1\leqslant L\leqslant 4$ for the Dirac one-electron atom in the ground state. The expressions for which $L\geqslant 2$ have been derived from Eq. (5.9).

L	$\sigma_{\mathrm{M}L\to\mathrm{M}L}$	Constraint on Z
1	$-\alpha^2Z\frac{2(4\gamma_1^3+6\gamma_1^2-7\gamma_1-12)}{27\gamma_1(\gamma_1+1)(2\gamma_1-1)}$	$Z<\alpha^{-1}\frac{\sqrt{3}}{2}$
2	$-\alpha^2Z\frac{8\gamma_1^3+58\gamma_1^2+133\gamma_1+71}{5(\gamma_1+1)(2\gamma_1+7)(4\gamma_1-1)}$	$Z<\alpha^{-1}\frac{\sqrt{15}}{4}$
3	$-\alpha^2Z\frac{2(48\gamma_1^5+964\gamma_1^4+7284\gamma_1^3+23887\gamma_1^2+33618\gamma_1+15199)}{35(\gamma_1+1)(\gamma_1+7)(2\gamma_1+7)(4\gamma_1+11)(6\gamma_1-1)}$	$Z<\alpha^{-1}\frac{\sqrt{35}}{6}$
4	$-\alpha^2Z\frac{2(128\gamma_1^7+5072\gamma_1^6+80580\gamma_1^5+636000\gamma_1^4+2680407\gamma_1^3+5997453\gamma_1^2+6535165\gamma_1+2587195)}{81(\gamma_1+1)(\gamma_1+5)(\gamma_1+7)(2\gamma_1+5)(2\gamma_1+23)(4\gamma_1+11)(8\gamma_1-1)}$	$Z<\alpha^{-1}\frac{3\sqrt{7}}{8}$

TABLE VIII. Quasirelativistic approximations for static magnetic multipole nuclear shielding constants $\sigma_{\mathrm{M}L\to\mathrm{M}L}$ with $1 \leqslant L \leqslant 4$ for the Dirac one-electron atom in the ground state. The expressions for which $L \geqslant 2$ have been derived from Eq. (5.11).

L	$\sigma_{\mathrm{M}L\to\mathrm{M}L}$
1	$\alpha^2 Z\,\frac{1}{3}[1+\frac{97}{36}(\alpha Z)^2]$
2	$-\alpha^2 Z\,[1+\frac{47}{90}(\alpha Z)^2]$
3	$-\alpha^2 Z\,\frac{3}{7}[1+\frac{5339}{10800}(\alpha Z)^2]$
4	$-\alpha^2 Z\,\frac{7}{27}[1+\frac{9521}{19600}(\alpha Z)^2]$

The quasirelativistic limit for the dipole shielding constant is easily found to be

$$\sigma_{\mathrm{M}1\to\mathrm{M}1} \simeq \alpha^2 Z\,\tfrac{1}{3}\big[1+\tfrac{97}{36}(\alpha Z)^2\big], \tag{5.10}$$

while that for $\sigma_{\mathrm{M}L\to\mathrm{M}L}$ with $L \geqslant 2$ is

$$\begin{aligned}\sigma_{\mathrm{M}L\to\mathrm{M}L} \simeq{}& -\alpha^2 Z\,\frac{L+3}{(L-1)(2L+1)}\bigg\{1-(\alpha Z)^2\\ &\times\frac{(L-1)(4L^2+5L+2)}{L(L+1)(L+2)(L+3)}\bigg[\psi(2L)-\psi(L)\\ &-\frac{L(L^3+11L^2+14L+6)}{2(L-1)(4L^2+5L+2)}\bigg]\bigg\}\quad (L\geqslant 2).\end{aligned} \tag{5.11}$$

The explicit forms of the quasirelativistic expressions approximating the shielding constants $\sigma_{\mathrm{M}L\to\mathrm{M}L}$ with $1 \leqslant L \leqslant 4$ are brought together in Table VIII. In the dipole case, our result agrees with those found in Refs. [7,19,20,31,32].[3] In the quadrupole and octupole cases, Refs. [19,20] give incorrect values for the factors R_L multiplying $(\alpha Z)^2$: for R_2 one should read 47/90 (= 705/1350) instead of 707/1350, while for R_3 the correct value is $5339/10800 \simeq 0.494$ rather than 0.292.

VI. NEAR-NUCLEUS ELECTRIC MULTIPOLE MOMENTS OF THE ATOM IN THE MULTIPOLE MAGNETIC FIELD AND NEAR-NUCLEUS ML → E($L \mp 1$) MULTIPOLE CROSS-SUSCEPTIBILITIES

Finally, we consider the near-field electric multipole moments R_λ, related, like their far-field counterparts Q_λ, to the electronic charge distribution $\rho(\boldsymbol{r})$ defined in Eq. (4.2). Spherical components of such moments are defined as

$$\mathcal{R}_{\lambda\mu} = \sqrt{\frac{4\pi}{2\lambda+1}}\int_{\mathbb{R}^3} d^3\boldsymbol{r}\; r^{-\lambda-1}Y_{\lambda\mu}(\boldsymbol{n}_r)\rho(\boldsymbol{r}). \tag{6.1}$$

If the charge density $\rho(\boldsymbol{r})$ is approximated as in Eq. (4.3), we have

$$\mathsf{R}_\lambda \simeq \mathsf{R}_\lambda^{(0)} + \mathsf{R}_\lambda^{(1)}, \tag{6.2}$$

with components of the moment tensors $\mathsf{R}_\lambda^{(0)}$ (the permanent one) and $\mathsf{R}_\lambda^{(1)}$ (the induced one) defined through the relations

$$\mathcal{R}_{\lambda\mu}^{(0)} = \sqrt{\frac{4\pi}{2\lambda+1}}\int_{\mathbb{R}^3} d^3\boldsymbol{r}\; r^{-\lambda-1}Y_{\lambda\mu}(\boldsymbol{n}_r)\rho^{(0)}(\boldsymbol{r}) \tag{6.3}$$

and

$$\mathcal{R}_{\lambda\mu}^{(1)} = \sqrt{\frac{4\pi}{2\lambda+1}}\int_{\mathbb{R}^3} d^3\boldsymbol{r}\; r^{-\lambda-1}Y_{\lambda\mu}(\boldsymbol{n}_r)\rho^{(1)}(\boldsymbol{r}). \tag{6.4}$$

The unperturbed and the first-order induced electronic charge densities $\rho^{(0)}(\boldsymbol{r})$ and $\rho^{(1)}(\boldsymbol{r})$ have been defined in Eqs. (4.4) and (4.5), respectively.

Evaluation of the integrals in Eqs. (6.3) and (6.4) casts Eq. (6.2) into the following one:

$$\mathsf{R}_\lambda \simeq \mathsf{R}_\lambda^{(0)}\delta_{\lambda 0} + \mathsf{R}_\lambda^{(1)}(\delta_{\lambda,L-1}+\delta_{\lambda,L+1}). \tag{6.5}$$

The only nonvanishing permanent moment from the family considered here is the monopole one, given by [10, Eq. (6.9)]

$$\mathcal{R}_{00}^{(0)} = -\frac{Ze}{\gamma_1 a_0}, \tag{6.6}$$

while the induced moments are of the form

$$\mathsf{R}_\lambda^{(1)} = (4\pi\epsilon_0)c\sigma_{\mathrm{M}L\to\mathrm{E}\lambda}\frac{\{\boldsymbol{\nu}\otimes\mathsf{D}_L^{(1)}\}_\lambda}{\langle 10;L0|\lambda 0\rangle}\quad(\lambda = L\mp 1). \tag{6.7}$$

The near-field magnetic-to-electric cross-susceptibilities $\sigma_{\mathrm{M}L\to\mathrm{E}(L\mp1)}$ are

$$\sigma_{\mathrm{M}1\to\mathrm{E}0} = \frac{\alpha a_0}{Z}\frac{\gamma_1^2-1}{3\gamma_1}\quad\left(= -\frac{\alpha a_0}{Z}\frac{(\alpha Z)^2}{3\gamma_1}\right), \tag{6.8}$$

$$\sigma_{\mathrm{M}L\to\mathrm{E}(L-1)} = \frac{\alpha a_0}{Z}\frac{L(2\gamma_1+1)}{(L-1)(4L^2-1)}\left\{1+\frac{(L^2-1)(\gamma_1+1)}{(\gamma_L-\gamma_1+1)(\gamma_L+\gamma_1-L+1)}\,{}_3F_2\left(\begin{matrix}-L+2,\,1,\,\gamma_L-\gamma_1-L\\ \gamma_L-\gamma_1+2,\,\gamma_L+\gamma_1-L+2\end{matrix};1\right)\right\}\quad(L\geqslant 2), \tag{6.9}$$

and

$$\begin{aligned}\sigma_{\mathrm{M}L\to\mathrm{E}(L+1)} ={}& \frac{\alpha Z}{a_0}\frac{2L}{\gamma_1(L+2)(2L+1)(2L+3)}\bigg\{1-\frac{(L+1)[\gamma_1(L+2)-L-1]}{(\gamma_{L+1}-\gamma_1+1)(\gamma_{L+1}+\gamma_1-L-1)}\\ &\times{}_3F_2\left(\begin{matrix}-L,\,1,\,\gamma_{L+1}-\gamma_1-L\\ \gamma_{L+1}-\gamma_1+2,\,\gamma_{L+1}+\gamma_1-L\end{matrix};1\right)\bigg\}\quad\left(Z<\alpha^{-1}\frac{\sqrt{(2L+1)(2L+3)}}{2(L+1)}\right).\end{aligned} \tag{6.10}$$

[3] There is a sign misprint in Ref. [20, Eq. (4.41)]: The factor $[1-(\alpha Z)^2 R_l]$ should be replaced by $[1+(\alpha Z)^2 R_l]$ (cf. Ref. [19]).

TABLE IX. Exact analytical expressions for the near-nucleus static magnetic-to-electric multipole cross-susceptibilities of the Dirac one-electron atom in the ground state. The expressions for $\sigma_{\mathrm{M}L\to\mathrm{E}(L-1)}$, derived from Eqs. (6.8) and (6.9), and given in the second column, are valid provided that $Z < \alpha^{-1}$. The last column displays constraints on the nuclear charge number Z under which the expressions for $\sigma_{\mathrm{M}L\to\mathrm{E}(L+1)}$ with $1 \leqslant L \leqslant 4$, obtained from Eq. (6.10) and given in the third column, remain valid.

L	$\sigma_{\mathrm{M}L\to\mathrm{E}(L-1)}$	$\sigma_{\mathrm{M}L\to\mathrm{E}(L+1)}$	Constraint on Z in $\sigma_{\mathrm{M}L\to\mathrm{E}(L+1)}$
1	$\frac{\alpha a_0}{Z}\frac{\gamma_1^2-1}{3\gamma_1} \quad (= -\frac{\alpha a_0}{Z}\frac{(\alpha Z)^2}{3\gamma_1})$	$\frac{(\alpha Z)^3}{a_0}\frac{2(8\gamma_1+3)}{45\gamma_1(\gamma_1+1)^2(4\gamma_1-1)}$	$Z < \alpha^{-1}\frac{\sqrt{15}}{4}$
2	$\frac{\alpha a_0}{Z}\frac{2\gamma_1+1}{3}$	$\frac{(\alpha Z)^3}{a_0}\frac{2(30\gamma_1^2+79\gamma_1+28)}{35\gamma_1(\gamma_1+1)^2(2\gamma_1+7)(6\gamma_1-1)}$	$Z < \alpha^{-1}\frac{\sqrt{35}}{6}$
3	$\frac{\alpha a_0}{Z}\frac{3(2\gamma_1+1)(2\gamma_1+5)}{14(2\gamma_1+7)}$	$\frac{(\alpha Z)^3}{a_0}\frac{2(96\gamma_1^3+684\gamma_1^2+1153\gamma_1+385)}{35\gamma_1(\gamma_1+1)^2(\gamma_1+7)(4\gamma_1+11)(8\gamma_1-1)}$	$Z < \alpha^{-1}\frac{3\sqrt{7}}{8}$
4	$\frac{\alpha a_0}{Z}\frac{2(2\gamma_1+1)(68\gamma_1^2+483\gamma_1+709)}{189(\gamma_1+7)(4\gamma_1+11)}$	$\frac{(\alpha Z)^3}{a_0}\frac{16(140\gamma_1^4+1976\gamma_1^3+8101\gamma_1^2+10870\gamma_1+3450)}{297\gamma_1(\gamma_1+1)^2(\gamma_1+5)(2\gamma_1+5)(2\gamma_1+23)(10\gamma_1-1)}$	$Z < \alpha^{-1}\frac{3\sqrt{11}}{10}$

Their explicit forms for $1 \leqslant L \leqslant 4$ are presented in Table IX. The quasirelativistic limits of Eqs. (6.8)–(6.10) are found to be

$$\sigma_{\mathrm{M}1\to\mathrm{E}0} \simeq -\frac{\alpha a_0}{Z}\frac{1}{3}(\alpha Z)^2, \tag{6.11}$$

$$\sigma_{\mathrm{M}L\to\mathrm{E}(L-1)} \simeq \frac{\alpha a_0}{Z}\frac{1}{L-1}\left\{1-(\alpha Z)^2\frac{L-1}{L}\left[\psi(2L)-\psi(L)-\frac{L(4L^2-3L-5)}{4(L-1)(4L^2-1)}\right]\right\} \quad (L \geqslant 2), \tag{6.12}$$

and

$$\sigma_{\mathrm{M}L\to\mathrm{E}(L+1)} \simeq \frac{\alpha Z}{a_0}(\alpha Z)^2\frac{2L^2}{(L+1)(L+2)(2L+1)(2L+3)}\left[\psi(2L+2)-\psi(L+1)+\frac{L+1}{2}\right], \tag{6.13}$$

respectively (cf. Table X for explicit forms of these approximations for $1 \leqslant L \leqslant 4$). We are not aware of any other studies on the susceptibilities of that kind.

TABLE X. Quasirelativistic approximations for the near-nucleus static magnetic-to-electric multipole cross-susceptibilities $\sigma_{\mathrm{M}L\to\mathrm{E}(L-1)}$ with $2 \leqslant L \leqslant 4$ and $\sigma_{\mathrm{M}L\to\mathrm{E}(L+1)}$ with $1 \leqslant L \leqslant 4$ for the Dirac one-electron atom in the ground state. The expressions have been derived from Eqs. (6.11)–(6.13).

L	$\sigma_{\mathrm{M}L\to\mathrm{E}(L-1)}$	$\sigma_{\mathrm{M}L\to\mathrm{E}(L+1)}$
1	$-\frac{\alpha a_0}{Z}\frac{1}{3}(\alpha Z)^2$	$\frac{(\alpha Z)^3}{a_0}\frac{11}{270}$
2	$\frac{\alpha a_0}{Z}[1-\frac{1}{3}(\alpha Z)^2]$	$\frac{(\alpha Z)^3}{a_0}\frac{137}{3150}$
3	$\frac{\alpha a_0}{Z}\frac{1}{2}[1-\frac{23}{63}(\alpha Z)^2]$	$\frac{(\alpha Z)^3}{a_0}\frac{1159}{29400}$
4	$\frac{\alpha a_0}{Z}\frac{1}{3}[1-\frac{1931}{5040}(\alpha Z)^2]$	$\frac{(\alpha Z)^3}{a_0}\frac{16358}{467775}$

VII. SUMMARY

On the preceding pages, we have investigated far- and near-field magnetic ($\mathbf{M}_L^{(1)}$ and $\mathbf{N}_L^{(1)}$) and electric ($\mathbf{Q}_{L\mp1}^{(1)}$ and $\mathbf{R}_{L\mp1}^{(1)}$) multipole moments induced in the ground state of the electronic cloud of the Dirac hydrogenlike atom by a weak static 2^L-pole magnetic field. For the reader's benefit, in Table XI we collect expressions relating the four moments listed above to the tensor $\mathbf{D}_L^{(1)}$ characterizing the strength and directional properties of the perturbing magnetic field; these formulas serve also as definitions of the corresponding atomic susceptibilities. Closed-form formulas for the atomic multipole magnetizabilities χ_L ($\equiv \chi_{\mathrm{M}L\to\mathrm{M}L}$), the far-field magnetic-to-electric cross-susceptibilities $\chi_{\mathrm{M}L\to\mathrm{E}(L\mp1)}$, the magnetic nuclear shielding constants $\sigma_{\mathrm{M}L\to\mathrm{M}L}$, and the near-nucleus magnetic-to-electric cross-susceptibilities $\sigma_{\mathrm{M}L\to\mathrm{E}(L\mp1)}$, derived in Secs. III–VI, are conveniently brought together in Tables XII and XIII. It is worth recalling here the important inference from Sec. IV that the magnetic-to-electric cross-susceptibilities $\chi_{\mathrm{M}L\to\mathrm{E}\lambda}$ are related to their electric-to-magnetic counterparts $\alpha_{\mathrm{E}L'\to\mathrm{M}\lambda'}$ through the identity $\chi_{\mathrm{M}L\to\mathrm{E}(L\mp1)} = \alpha_{\mathrm{E}(L\mp1)\to\mathrm{M}L}$.

In our previous paper [10], where we have dealt with the atomic response to an external multipole electric field, in addition to the moments $\mathbf{M}_L^{(1)}$, $\mathbf{N}_L^{(1)}$, $\mathbf{Q}_{L\mp1}^{(1)}$, and $\mathbf{R}_{L\mp1}^{(1)}$ we have also studied the electric-field-induced far- and near-field multipole toroidal magnetic moments $\mathbf{T}_\lambda^{(1)}$ and $\mathbf{U}_\lambda^{(1)}$ (cf. Secs. V and VIII, as well as Appendixes C and D in Ref. [10]), with components

$$\mathcal{T}_{\lambda\mu}^{(1)} = \frac{1}{\lambda+1}\sqrt{\frac{4\pi}{2\lambda+1}}\int_{\mathbb{R}^3} d^3\boldsymbol{r}\, r^\lambda Y_{\lambda\mu}(\boldsymbol{n}_r)\boldsymbol{r}\cdot\boldsymbol{j}^{(1)}(\boldsymbol{r}) \tag{7.1}$$

and

$$\mathcal{U}_{\lambda\mu}^{(1)} = -\frac{1}{\lambda}\sqrt{\frac{4\pi}{2\lambda+1}}\int_{\mathbb{R}^3} d^3\boldsymbol{r}\, r^{-\lambda-1} Y_{\lambda\mu}(\boldsymbol{n}_r)\boldsymbol{r}\cdot\boldsymbol{j}^{(1)}(\boldsymbol{r}), \tag{7.2}$$

respectively; we have found that the only nonvanishing moments of such sorts are those for which $\lambda = L$. We have not deliberated on these two families of moments in the present paper, since if the perturbing field is the magnetic one, the right-hand sides of Eqs. (7.1) and (7.2) are found to vanish whatever the value of λ is, in result of integrations over angular variables.

For the sake of completeness of the present study, we include here still one more table, Table XIV, to show how the susceptibilities investigated in this work enter the near- and far-zone asymptotic representations of electric and magnetic

TABLE XI. The collection of formulas defining the multipole susceptibilities considered in the present paper.

Susceptibility	Related induced moment	Constraints
	Far-field zone	
$\chi_{ML\to ML}$	$\mathbf{M}_L^{(1)} = (\frac{\mu_0}{4\pi})^{-1}\chi_{ML\to ML}\,\mathbf{D}_L^{(1)}$	
$\chi_{ML\to E\lambda}$	$\mathbf{Q}_\lambda^{(1)} = (\frac{\mu_0}{4\pi})^{-1}c^{-1}\chi_{ML\to E\lambda}\frac{\{\boldsymbol{\nu}\otimes\mathbf{D}_L^{(1)}\}_\lambda}{\langle 10;L0\|\lambda 0\rangle}$	$\lambda = \begin{cases}2 & \text{for } L=1\\ L\mp 1 & \text{for L} \geqslant 2\end{cases}$
	Near-nucleus zone	
$\sigma_{ML\to ML}$	$\mathbf{N}_L^{(1)} = (\frac{\mu_0}{4\pi})^{-1}\sigma_{ML\to ML}\,\mathbf{D}_L^{(1)}$	
$\sigma_{ML\to E\lambda}$	$\mathbf{R}_\lambda^{(1)} = (\frac{\mu_0}{4\pi})^{-1}c^{-1}\sigma_{ML\to E\lambda}\frac{\{\boldsymbol{\nu}\otimes\mathbf{D}_L^{(1)}\}_\lambda}{\langle 10;L0\|\lambda 0\rangle}$	$\lambda = L\mp 1$

fields (and of their potentials), which are due to the first-order changes in the electronic charge and current densities induced by the perturbing external magnetic field.

Two further important results concerning the multipole magnetizabilities $\chi_L \equiv \chi_{ML\to ML}$ and the far-field cross-susceptibilities $\chi_{ML_2\to EL_1} = \alpha_{EL_1\to ML_2}$ are presented below in Appendixes B and C, respectively. In Appendix B, we establish a relationship between the second-order energy correction $E^{(2)}$, the magnetizability χ_L and the tensor $\mathbf{D}_L^{(1)}$ characterizing the magnetic field which perturbs the ground state of the atom; in fact, this relationship may serve as a definition of the magnetizability χ_L which is alternative, but still equivalent, to the one given in Sec. III and in Table XI. In turn, in Appendix C we consider the ground state of the atom subjected to the simultaneous action of the perturbing 2^{L_1}-pole electric and 2^{L_2}-pole magnetic fields. We show that if $L_2 \neq L_1 \mp 1$, then both types of fields contribute independently to the second-order energy correction $E^{(2)}$. If, however, the constraint $L_2 = L_1 \mp 1$ is imposed, then an additional mixed electromagnetic contribution to $E^{(2)}$ arises, which involves the cross-susceptibility $\alpha_{EL_1\to ML_2} = \chi_{ML_2\to EL_1}$. This implies the positive answer to the quite natural question whether the far-field cross-susceptibilities investigated here and in Ref. [10] are measurable quantities.

ACKNOWLEDGMENT

We thank Dr. Patrycja Stefańska for valuable discussions.

APPENDIX A: SOME RELEVANT SUMS OVER MAGNETIC QUANTUM NUMBERS

Throughout this Appendix, the symbols $\mathbf{A}_L$ and $\mathbf{B}_{L'}$ denote two spherical tensor operators of integer ranks L and L', respectively, components of which obey

$$\mathcal{A}^*_{LM} = (-)^M\mathcal{A}_{L,-M}, \quad \mathcal{B}^*_{L'M'} = (-)^{M'}\mathcal{B}_{L',-M'}. \tag{A1}$$

1. Triple sums

The following formulas for triple sums over magnetic quantum numbers hold:

$$\begin{aligned}
&\sum_{M=-L}^{L}\sum_{M'=-L'}^{L'}\sum_{m_\kappa=-|\kappa|+1/2}^{|\kappa|-1/2}\mathcal{A}^*_{LM}\mathcal{B}^*_{L'M'}\langle\Omega_{-1m}|Y_{LM}\Omega_{\kappa m_\kappa}\rangle\langle\Omega_{\kappa m_\kappa}|Y_{L'M'}\Omega_{-1m'}\rangle\\
&= \delta_{LL'}(\delta_{\kappa L}+\delta_{\kappa,-L-1})\frac{(-)^L}{4\pi\sqrt{2L+1}}\bigg\{(\delta_{m,1/2}\delta_{m',1/2}+\delta_{m,-1/2}\delta_{m',-1/2})|\kappa|\{\mathbf{A}_L\otimes\mathbf{B}_{L'}\}_{00}\\
&\quad-\operatorname{sgn}(\kappa)\sqrt{\frac{L(L+1)}{3}}[\delta_{m,1/2}\delta_{m',1/2}\{\mathbf{A}_L\otimes\mathbf{B}_{L'}\}_{10}+\delta_{m,1/2}\delta_{m',-1/2}\sqrt{2}\{\mathbf{A}_L\otimes\mathbf{B}_{L'}\}_{1,-1}\\
&\quad-\delta_{m,-1/2}\delta_{m',1/2}\sqrt{2}\{\mathbf{A}_L\otimes\mathbf{B}_{L'}\}_{11}-\delta_{m,-1/2}\delta_{m',-1/2}\{\mathbf{A}_L\otimes\mathbf{B}_{L'}\}_{10}]\bigg\},
\end{aligned}\tag{A2}$$

$$\begin{aligned}
&\sum_{M=-L}^{L}\sum_{M'=-L'}^{L'}\sum_{m_\kappa=-|\kappa|+1/2}^{|\kappa|-1/2}\mathcal{A}^*_{LM}\mathcal{B}^*_{L'M'}\langle\Omega_{-1m}|Y_{LM}\Omega_{\kappa m_\kappa}\rangle\langle\Omega_{-\kappa m_\kappa}|Y_{L'M'}\Omega_{-1m'}\rangle\\
&= -(\delta_{\kappa L}\delta_{\kappa,L'+1}+\delta_{\kappa,-L-1}\delta_{\kappa,-L'})\frac{|\kappa|}{4\pi\sqrt{(2L+1)(2L'+1)}\,\langle L0;L'0|10\rangle}[\delta_{m,1/2}\delta_{m',1/2}\{\mathbf{A}_L\otimes\mathbf{B}_{L'}\}_{10}\\
&\quad+\delta_{m,1/2}\delta_{m',-1/2}\sqrt{2}\{\mathbf{A}_L\otimes\mathbf{B}_{L'}\}_{1,-1}-\delta_{m,-1/2}\delta_{m',1/2}\sqrt{2}\{\mathbf{A}_L\otimes\mathbf{B}_{L'}\}_{11}-\delta_{m,-1/2}\delta_{m',-1/2}\{\mathbf{A}_L\otimes\mathbf{B}_{L'}\}_{10}].
\end{aligned}\tag{A3}$$

Here

$$\{\mathbf{A}_L\otimes\mathbf{B}_{L'}\}_{JM_J} = \sum_{M=-L}^{L}\sum_{M'=-L'}^{L'}\langle LM;L'M'|JM_J\rangle\mathcal{A}_{LM}\mathcal{B}_{L'M'}, \tag{A4}$$

TABLE XII. The collection of exact analytical expressions for the far-field static magnetic multipole susceptibilities for the Dirac one-electron atom in the ground state: the magnetizability $\chi_{\mathrm{M}L\to\mathrm{M}L}$ ($\equiv\chi_L$) and the magnetic-to-electric cross-susceptibilities $\chi_{\mathrm{M}L\to\mathrm{E}(L\mp1)}$. All the formulas are valid under the constraint $Z<\alpha^{-1}$.

Susceptibility	Constraints
$\chi_{\mathrm{M1}\to\mathrm{M1}} = -\frac{\alpha^2 a_0^3}{Z^2}\frac{(\gamma_1+1)(4\gamma_1^2-1)}{18}\left\{1+\frac{(\gamma_2+\gamma_1)\Gamma^2(\gamma_2+\gamma_1+2)}{6(2\gamma_1-1)\Gamma(2\gamma_1+3)\Gamma(2\gamma_2+1)}\,{}_3F_2\left(\begin{matrix}\gamma_2-\gamma_1-1,\gamma_2-\gamma_1-1,\gamma_2-\gamma_1\\ \gamma_2-\gamma_1+1,2\gamma_2+1\end{matrix};1\right)\right\}$	
$\chi_{\mathrm{M}L\to\mathrm{M}L} = \frac{\alpha^2 a_0^{2L+1}}{Z^{2L}}\frac{L}{2^{2L}(L+1)(2L+1)^2\Gamma(2\gamma_1+1)}\left\{\frac{(L+1)^2\Gamma^2(\gamma_L+\gamma_1+L+1)}{(\gamma_L-\gamma_1)\Gamma(2\gamma_L+1)}\,{}_3F_2\left(\begin{matrix}\gamma_L-\gamma_1-L,\ \gamma_L-\gamma_1-L,\ \gamma_L-\gamma_1\\ \gamma_L-\gamma_1+1,\ 2\gamma_L+1\end{matrix};1\right)\right.$ $\left.-\frac{L^2\Gamma^2(\gamma_{L+1}+\gamma_1+L+1)}{(\gamma_{L+1}-\gamma_1)\Gamma(2\gamma_{L+1}+1)}\,{}_3F_2\left(\begin{matrix}\gamma_{L+1}-\gamma_1-L,\ \gamma_{L+1}-\gamma_1-L,\ \gamma_{L+1}-\gamma_1\\ \gamma_{L+1}-\gamma_1+1,\ 2\gamma_{L+1}+1\end{matrix};1\right)\right\}$	$L\geqslant 2$
$\chi_{\mathrm{M}L\to\mathrm{E}(L-1)} = \frac{\alpha a_0^{2L}}{Z^{2L}}\frac{L\Gamma(2\gamma_1+2L+1)}{2^{2L-1}(L-1)(4L^2-1)\Gamma(2\gamma_1+1)}\left\{1+\frac{(L+1)[\gamma_1(L-1)-L]\Gamma(\gamma_L+\gamma_1+L)\Gamma(\gamma_L+\gamma_1+L+1)}{(\gamma_L-\gamma_1+1)\Gamma(2\gamma_1+2L+1)\Gamma(2\gamma_L+1)}\right.$ $\left.\times\,{}_3F_2\left(\begin{matrix}\gamma_L-\gamma_1-L,\ \gamma_L-\gamma_1-L+1,\ \gamma_L-\gamma_1+1\\ \gamma_L-\gamma_1+2,\ 2\gamma_L+1\end{matrix};1\right)\right\}$	$L\geqslant 2$
$\chi_{\mathrm{M}L\to\mathrm{E}(L+1)} = \frac{\alpha a_0^{2L+2}}{Z^{2L+2}}\frac{L\Gamma(2\gamma_1+2L+3)}{2^{2L+1}(L+2)(2L+1)(2L+3)\Gamma(2\gamma_1+1)}\left\{1-\frac{(L+1)(L+2)(\gamma_1+1)\Gamma(\gamma_{L+1}+\gamma_1+L+1)\Gamma(\gamma_{L+1}+\gamma_1+L+2)}{(\gamma_{L+1}-\gamma_1+1)\Gamma(2\gamma_1+2L+3)\Gamma(2\gamma_{L+1}+1)}\right.$ $\left.\times\,{}_3F_2\left(\begin{matrix}\gamma_{L+1}-\gamma_1-L-1,\ \gamma_{L+1}-\gamma_1-L,\ \gamma_{L+1}-\gamma_1+1\\ \gamma_{L+1}-\gamma_1+2,\ 2\gamma_{L+1}+1\end{matrix};1\right)\right\}$	

TABLE XIII. The collection of exact analytical expressions for the near-nucleus static magnetic multipole susceptibilities for the Dirac one-electron atom in the ground state: the magnetic nuclear shielding constant $\sigma_{\mathrm{M}L\to\mathrm{M}L}$ and the magnetic-to-electric cross-susceptibilities $\sigma_{\mathrm{M}L\to\mathrm{E}(L\mp1)}$.

Susceptibility	Constraints
$\sigma_{\mathrm{M1}\to\mathrm{M1}} = -\alpha^2 Z\frac{2(4\gamma_1^3+6\gamma_1^2-7\gamma_1-12)}{27\gamma_1(\gamma_1+1)(2\gamma_1-1)}$	$Z<\alpha^{-1}\frac{\sqrt{3}}{2}$
$\sigma_{\mathrm{M}L\to\mathrm{M}L} = -\alpha^2 Z\frac{2}{(2L+1)^2}\left\{\frac{(L+1)^2}{(\gamma_L-\gamma_1)(\gamma_L+\gamma_1-L)}\,{}_3F_2\left(\begin{matrix}-L,\ 1,\ \gamma_L-\gamma_1-L\\ \gamma_L-\gamma_1+1,\ \gamma_L+\gamma_1-L+1\end{matrix};1\right)\right.$ $\left.-\frac{L^2}{(\gamma_{L+1}-\gamma_1)(\gamma_{L+1}+\gamma_1-L)}\,{}_3F_2\left(\begin{matrix}-L,\ 1,\ \gamma_{L+1}-\gamma_1-L\\ \gamma_{L+1}-\gamma_1+1,\ \gamma_{L+1}+\gamma_1-L+1\end{matrix};1\right)\right\}$	$L\geqslant 2$; $Z<\alpha^{-1}\frac{\sqrt{4L^2-1}}{2L}$
$\sigma_{\mathrm{M1}\to\mathrm{E0}} = \frac{\alpha a_0}{Z}\frac{\gamma_1^2-1}{3\gamma_1}\quad\left(=-\frac{\alpha a_0}{Z}\frac{(\alpha Z)^2}{3\gamma_1}\right)$	
$\sigma_{\mathrm{M}L\to\mathrm{E}(L-1)} = \frac{\alpha a_0}{Z}\frac{L(2\gamma_1+1)}{(L-1)(4L^2-1)}\left\{1+\frac{(L^2-1)(\gamma_1+1)}{(\gamma_L-\gamma_1+1)(\gamma_L+\gamma_1-L+1)}\,{}_3F_2\left(\begin{matrix}-L+2,\ 1,\ \gamma_L-\gamma_1-L\\ \gamma_L-\gamma_1+2,\ \gamma_L+\gamma_1-L+2\end{matrix};1\right)\right\}$	$L\geqslant 2$
$\sigma_{\mathrm{M}L\to\mathrm{E}(L+1)} = \frac{\alpha Z}{a_0}\frac{2L}{\gamma_1(L+2)(2L+1)(2L+3)}\left\{1-\frac{(L+1)[\gamma_1(L+2)-L-1]}{(\gamma_{L+1}-\gamma_1+1)(\gamma_{L+1}+\gamma_1-L-1)}\,{}_3F_2\left(\begin{matrix}-L,\ 1,\ \gamma_{L+1}-\gamma_1-L\\ \gamma_{L+1}-\gamma_1+2,\ \gamma_{L+1}+\gamma_1-L\end{matrix};1\right)\right\}$	$Z<\alpha^{-1}\frac{\sqrt{(2L+1)(2L+3)}}{2(L+1)}$

TABLE XIV. The table shows how the susceptibilities studied in the present paper enter the near- and far-zone asymptotic representations of static electric $\boldsymbol{E}^{(1)}(\boldsymbol{r})$ and magnetic $\boldsymbol{B}^{(1)}(\boldsymbol{r})$ fields, and of their potentials: scalar $\phi^{(1)}(\boldsymbol{r})$ and vector $\boldsymbol{A}^{(1)}(\boldsymbol{r})$, which are due to the first-order charge and current densities induced in the ground state of the hydrogenic atom by an external 2^L-pole ($L \geqslant 1$) static magnetic field $\boldsymbol{\mathcal{B}}_L^{(1)}(\boldsymbol{r})$ given in Eq. (2.2) and derived from the vector potential $\boldsymbol{\mathcal{A}}_L^{(1)}(\boldsymbol{r})$ defined in Eq. (2.1).

Induced field	Near-zone representation	Far-zone representation
$\phi^{(1)}(\boldsymbol{r})$	$\sum_{\lambda=L\mp1} c\sigma_{\mathrm{ML}\to\mathrm{E}\lambda}\sqrt{\frac{4\pi}{2\lambda+1}}\, r^{\lambda}\sum_{\mu=-\lambda}^{\lambda}\frac{\{\boldsymbol{\nu}\otimes\mathbf{D}_L^{(1)}\}_{\lambda\mu}}{\langle 10;L0\|\lambda0\rangle}Y_{\lambda\mu}^{*}(\boldsymbol{n}_r)$	$\sum_{\substack{\lambda=L\mp1\\(\lambda\neq0)}} c\chi_{\mathrm{ML}\to\mathrm{E}\lambda}\sqrt{\frac{4\pi}{2\lambda+1}}\, r^{-\lambda-1}\sum_{\mu=-\lambda}^{\lambda}\frac{\{\boldsymbol{\nu}\otimes\mathbf{D}_L^{(1)}\}_{\lambda\mu}}{\langle 10;L0\|\lambda0\rangle}Y_{\lambda\mu}^{*}(\boldsymbol{n}_r)$
$\boldsymbol{E}^{(1)}(\boldsymbol{r})$	$-\sum_{\substack{\lambda=L\mp1\\(\lambda\neq0)}} c\sigma_{\mathrm{ML}\to\mathrm{E}\lambda}\sqrt{4\pi\lambda}\, r^{\lambda-1}\sum_{\mu=-\lambda}^{\lambda}\frac{\{\boldsymbol{\nu}\otimes\mathbf{D}_L^{(1)}\}_{\lambda\mu}}{\langle 10;L0\|\lambda0\rangle}\boldsymbol{Y}_{\lambda\mu}^{\lambda-1*}(\boldsymbol{n}_r)$	$-\sum_{\substack{\lambda=L\mp1\\(\lambda\neq0)}} c\chi_{\mathrm{ML}\to\mathrm{E}\lambda}\sqrt{4\pi(\lambda+1)}\, r^{-\lambda-2}\sum_{\mu=-\lambda}^{\lambda}\frac{\{\boldsymbol{\nu}\otimes\mathbf{D}_L^{(1)}\}_{\lambda\mu}}{\langle 10;L0\|\lambda0\rangle}\boldsymbol{Y}_{\lambda\mu}^{\lambda+1*}(\boldsymbol{n}_r)$
$\boldsymbol{A}^{(1)}(\boldsymbol{r})$	$-i\sigma_{\mathrm{ML}\to\mathrm{ML}}\sqrt{\frac{4\pi L}{(L+1)(2L+1)}}\, r^{L}\sum_{M=-L}^{L}\mathcal{D}_{LM}^{(1)}\boldsymbol{Y}_{LM}^{L*}(\boldsymbol{n}_r) = -\sigma_{\mathrm{ML}\to\mathrm{ML}}\boldsymbol{\mathcal{A}}_L^{(1)}(\boldsymbol{r})$	$i\chi_{\mathrm{ML}\to\mathrm{ML}}\sqrt{\frac{4\pi(L+1)}{L(2L+1)}}\, r^{-L-1}\sum_{M=-L}^{L}\mathcal{D}_{LM}^{(1)}\boldsymbol{Y}_{LM}^{L*}(\boldsymbol{n}_r)$
$\boldsymbol{B}^{(1)}(\boldsymbol{r})$	$-\sigma_{\mathrm{ML}\to\mathrm{ML}}\sqrt{4\pi L}\, r^{L-1}\sum_{M=-L}^{L}\mathcal{D}_{LM}^{(1)}\boldsymbol{Y}_{LM}^{L-1*}(\boldsymbol{n}_r) = -\sigma_{\mathrm{ML}\to\mathrm{ML}}\boldsymbol{\mathcal{B}}_L^{(1)}(\boldsymbol{r})$	$-\chi_{\mathrm{ML}\to\mathrm{ML}}\sqrt{4\pi(L+1)}\, r^{-L-2}\sum_{M=-L}^{L}\mathcal{D}_{LM}^{(1)}\boldsymbol{Y}_{LM}^{L+1*}(\boldsymbol{n}_r)$

where $\langle j_1m_1; j_2m_2|j_3m_3\rangle$ is the Clebsch-Gordan coefficient, is an M_J component of the irreducible tensor product of rank J of $\mathbf{A}_L$ and $\mathbf{B}_{L'}$. For $L' = L$ and $\mathbf{B}_L = \mathbf{A}_L$, it holds that [21, Sec. 3.1.8]

$$\{\mathbf{A}_L \otimes \mathbf{A}_L\}_{00} = \frac{(-)^L}{\sqrt{2L+1}}\mathbf{A}_L \cdot \mathbf{A}_L, \tag{A5}$$

where

$$\mathbf{A}_L \cdot \mathbf{A}_L = \sum_{M=-L}^{L} |\mathcal{A}_{LM}|^2 \tag{A6}$$

is the scalar product of the tensor $\mathbf{A}_L$ with itself; moreover, one has

$$\{\mathbf{A}_L \otimes \mathbf{A}_L\}_{1M_J} = 0 \quad (M_J = 0,\pm1), \tag{A7}$$

and consequently Eq. (A2) simplifies to

$$\begin{aligned}
&\sum_{M=-L}^{L}\sum_{M'=-L}^{L}\sum_{m_\kappa=-|\kappa|+1/2}^{|\kappa|-1/2}\mathcal{A}_{LM}^{*}\mathcal{A}_{LM'}^{*}\\
&\quad\times\big\langle\Omega_{-1m}\big|Y_{LM}\Omega_{\kappa m_\kappa}\big\rangle\big\langle\Omega_{\kappa m_\kappa}\big|Y_{LM'}\Omega_{-1m'}\big\rangle\\
&\quad=(\delta_{\kappa L}+\delta_{\kappa,-L-1})(\delta_{m,1/2}\delta_{m',1/2}+\delta_{m,-1/2}\delta_{m',-1/2})\\
&\quad\times\frac{|\kappa|}{4\pi(2L+1)}\mathbf{A}_L\cdot\mathbf{A}_L.
\end{aligned}\tag{A8}$$

2. Quadruple sums

If the coefficients $a_{\pm1/2}$ satisfy the constraint

$$|a_{1/2}|^2 + |a_{-1/2}|^2 = 1, \tag{A9}$$

the following formulas involving quadruple sums over magnetic quantum numbers hold:

$$\begin{aligned}
&\sum_{M'=-L'}^{L'}\sum_{m=-1/2}^{1/2}\sum_{m'=-1/2}^{1/2}\sum_{m_\kappa=-|\kappa|+1/2}^{|\kappa|-1/2}\mathcal{B}_{L'M'}^{*}a_m^{*}a_{m'}\\
&\quad\times\big\langle\Omega_{-1m}\big|Y_{LM}\Omega_{\kappa m_\kappa}\big\rangle\big\langle\Omega_{\kappa m_\kappa}\big|Y_{L'M'}\Omega_{-1m'}\big\rangle\\
&\quad=\delta_{LL'}(\delta_{\kappa L}+\delta_{\kappa,-L-1})\frac{1}{4\pi(2L+1)}\\
&\quad\times[|\kappa|\mathcal{B}_{L'M}-\mathrm{sgn}(\kappa)\sqrt{L(L+1)}\{\boldsymbol{\nu}\otimes\mathbf{B}_{L'}\}_{L'M}],
\end{aligned}\tag{A10}$$

$$\begin{aligned}
&\sum_{M'=-L'}^{L'}\sum_{m=-1/2}^{1/2}\sum_{m'=-1/2}^{1/2}\sum_{m_\kappa=-|\kappa|+1/2}^{|\kappa|-1/2}\mathcal{B}_{L'M'}^{*}a_m^{*}a_{m'}\\
&\quad\times\big\langle\Omega_{-1m}\big|Y_{LM}\Omega_{\kappa m_\kappa}\big\rangle\big\langle\Omega_{-\kappa m_\kappa}\big|Y_{L'M'}\Omega_{-1m'}\big\rangle\\
&\quad=(\delta_{\kappa L}\delta_{\kappa,L'+1}+\delta_{\kappa,-L-1}\delta_{\kappa,-L'})\frac{1}{4\pi}\langle L0;10|L'0\rangle\\
&\quad\times\{\boldsymbol{\nu}\otimes\mathbf{B}_{L'}\}_{LM},
\end{aligned}\tag{A11}$$

where $\boldsymbol{\nu}$ is the unit vector with the cyclic components

$$\nu_0 = |a_{1/2}|^2 - |a_{-1/2}|^2, \quad \nu_{\pm1} = \mp\sqrt{2}\,a_{\pm1/2}^{*}a_{\mp1/2}. \tag{A12}$$

3. Quintuple sums

Provided the coefficients $a_{\pm 1/2}$ satisfy the constraint (A9), the following formulas for the quintuple sums over magnetic quantum numbers:

$$\sum_{M=-L}^{L}\sum_{M'=-L'}^{L'}\sum_{m=-1/2}^{1/2}\sum_{m'=-1/2}^{1/2}\sum_{m_\kappa=-|\kappa|+1/2}^{|\kappa|-1/2}\mathcal{A}_{LM}^{*}\mathcal{B}_{L'M'}^{*}a_m^{*}a_{m'}\langle\Omega_{-1m}|Y_{LM}\Omega_{\kappa m_\kappa}\rangle\langle\Omega_{\kappa m_\kappa}|Y_{L'M'}\Omega_{-1m'}\rangle$$
$$=\delta_{LL'}(\delta_{\kappa L}+\delta_{\kappa,-L-1})\frac{(-)^L}{4\pi\sqrt{2L+1}}\left[|\kappa|\{\mathbf{A}_L\otimes\mathbf{B}_{L'}\}_{00}-\mathrm{sgn}(\kappa)\sqrt{\frac{L(L+1)}{3}}\,\boldsymbol{\nu}\cdot\{\mathbf{A}_L\otimes\mathbf{B}_{L'}\}_1\right] \tag{A13}$$

and

$$\sum_{M=-L}^{L}\sum_{M'=-L'}^{L'}\sum_{m=-1/2}^{1/2}\sum_{m'=-1/2}^{1/2}\sum_{m_\kappa=-|\kappa|+1/2}^{|\kappa|-1/2}\mathcal{A}_{LM}^{*}\mathcal{B}_{L'M'}^{*}a_m^{*}a_{m'}\langle\Omega_{-1m}|Y_{LM}\Omega_{\kappa m_\kappa}\rangle\langle\Omega_{-\kappa m_\kappa}|Y_{L'M'}\Omega_{-1m'}\rangle$$
$$=-(\delta_{\kappa L}\delta_{\kappa,L'+1}+\delta_{\kappa,-L-1}\delta_{\kappa,-L'})\frac{|\kappa|}{4\pi\sqrt{(2L+1)(2L'+1)}}\frac{\boldsymbol{\nu}\cdot\{\mathbf{A}_L\otimes\mathbf{B}_{L'}\}_1}{\langle L0;L'0|10\rangle} \tag{A14}$$

may be derived from the pair of Eqs. (A2) and (A3) or, alternatively, from the pair of Eqs. (A10) and (A11). In both Eqs. (A13) and (A14), $\boldsymbol{\nu}$ is the vector with the cyclic components (A12). For $L'=L$ and $\mathbf{B}_L=\mathbf{A}_L$, by virtue of the identities (A5) and (A6), Eq. (A13) becomes

$$\sum_{M=-L}^{L}\sum_{M'=-L'}^{L'}\sum_{m=-1/2}^{1/2}\sum_{m'=-1/2}^{1/2}\sum_{m_\kappa=-|\kappa|+1/2}^{|\kappa|-1/2}\mathcal{A}_{LM}^{*}\mathcal{A}_{LM'}^{*}a_m^{*}a_{m'}\langle\Omega_{-1m}|Y_{LM}\Omega_{\kappa m_\kappa}\rangle\langle\Omega_{\kappa m_\kappa}|Y_{LM'}\Omega_{-1m'}\rangle$$
$$=(\delta_{\kappa L}+\delta_{\kappa,-L-1})\frac{|\kappa|}{4\pi(2L+1)}\mathbf{A}_L\cdot\mathbf{A}_L. \tag{A15}$$

APPENDIX B: MULTIPOLE MAGNETIZABILITIES VS THE SECOND-ORDER CORRECTION TO THE ATOMIC GROUND-STATE ENERGY

Within the framework of the second-order perturbation theory, the wave function and the energy eigenvalue are approximated as

$$\Psi(\boldsymbol{r})\simeq\Psi^{(0)}(\boldsymbol{r})+\Psi^{(1)}(\boldsymbol{r})+\Psi^{(2)}(\boldsymbol{r}) \tag{B1}$$

and

$$E\simeq E^{(0)}+E^{(1)}+E^{(2)}, \tag{B2}$$

respectively. The corrections $\Psi^{(2)}(\boldsymbol{r})$ and $E^{(2)}$ enter the inhomogeneous equation

$$\left[-ic\hbar\boldsymbol{\alpha}\cdot\nabla+\beta m_{\mathrm{e}}c^2-\frac{Ze^2}{(4\pi\epsilon_0)r}-E^{(0)}\right]\Psi^{(2)}(\boldsymbol{r})=-\left[V_L^{(1)}(\boldsymbol{r})-E^{(1)}\right]\Psi^{(1)}(\boldsymbol{r})+E^{(2)}\Psi^{(0)}(\boldsymbol{r}), \tag{B3}$$

which is to be solved subject to the usual regularity constraints, including the limit conditions

$$\lim_{r\to 0}r\Psi^{(2)}(\boldsymbol{r})=0,\quad \lim_{r\to\infty}r^{3/2}\Psi^{(2)}(\boldsymbol{r})=0, \tag{B4}$$

and also the orthogonality restraints

$$\int_{\mathbb{R}^3}d^3\boldsymbol{r}\;\Psi_m^{(0)\dagger}(\boldsymbol{r})\Psi^{(2)}(\boldsymbol{r})=0\quad\left(m=\pm\frac{1}{2}\right). \tag{B5}$$

For $L=1$, we know from Sec. II that the degeneracy of the atomic ground state is lifted already in the lowest order of the perturbation theory. There are two distinct first-order corrections $E_\pm^{(1)}$ to energy, given by Eq. (2.35), the related perturbation-adapted zeroth-order wave functions being the ones in Eq. (2.15) with the mixing coefficients (2.40). Hence, if we identify $\Psi^{(0)}(\boldsymbol{r})$ in Eq. (B3) either with $\Psi_+^{(0)}(\boldsymbol{r})$ (for the state with $E^{(1)}=E_+^{(1)}$) or with $\Psi_-^{(0)}(\boldsymbol{r})$ (for the state with $E^{(1)}=E_-^{(1)}$), then project the latter equation from the left onto the function chosen, after exploiting the orthogonality constraint (2.21) and the representation for $\Psi^{(1)}(\boldsymbol{r})$ displayed in Eq. (2.43) [again with $\Psi^{(0)}(\boldsymbol{r})$ identified with $\Psi_\pm^{(0)}(\boldsymbol{r})$], we obtain the corrections $E_\pm^{(2)}$ to $E^{(0)}+E_\pm^{(1)}$ in the form

$$E_\pm^{(2)}=-\int_{\mathbb{R}^3}d^3\boldsymbol{r}\int_{\mathbb{R}^3}d^3\boldsymbol{r}'\;\Psi_\pm^{(0)\dagger}(\boldsymbol{r})V_1^{(1)}(\boldsymbol{r})\bar{G}^{(0)}(\boldsymbol{r},\boldsymbol{r}')V_1^{(1)}(\boldsymbol{r}')\Psi_\pm^{(0)}(\boldsymbol{r}')\quad(L=1,\;E^{(1)}=E_\pm^{(1)}). \tag{B6}$$

After integrations over angular variables are done, Eq. (B6) goes over into

$$E^{(2)} = -\left(\frac{\mu_0}{4\pi}\right)^{-1}\left[\frac{1}{9}R_{-1}^{(1,1)}(Q^{(0)},P^{(0)};Q^{(0)},P^{(0)}) + \frac{1}{18}R_{2}^{(1,1)}(Q^{(0)},P^{(0)};Q^{(0)},P^{(0)})\right]\mathbf{D}_1^{(1)}\cdot\mathbf{D}_1^{(1)} \quad (L=1), \tag{B7}$$

with $R_\kappa^{(L_1,L_2)}(F_a,F_b;F_c,F_d)$ defined in Eq. (3.19). The right-hand side of Eq. (B7) is independent of which of the two levels which have arisen within the first-order perturbation theory is investigated; therefore, the subscript at $E^{(2)}$ has been dropped.

For $L \geqslant 2$, we know, again from Sec. II, that the first-order energy correction is zero, and therefore the perturbation-adapted zeroth-order wave function in Eq. (B3) is the one given by Eq. (2.14), with the mixing coefficients $a_{\pm 1/2}$ chosen at will [up to the normalization constraint (2.19)]. Projecting then Eq. (B3) onto the basis functions $\Psi_{\pm 1/2}^{(0)}(\boldsymbol{r})$ leads to the algebraic 2×2 system

$$\sum_{m'=-1/2}^{1/2}\left[V_{L,mm'}^{(1,1)} - E^{(2)}\delta_{mm'}\right]a_{m'} = 0 \quad \left(m = \pm\frac{1}{2},\ L \geqslant 2\right), \tag{B8}$$

where

$$V_{L,mm'}^{(1,1)} = -\int_{\mathbb{R}^3} d^3\boldsymbol{r}\int_{\mathbb{R}^3} d^3\boldsymbol{r}'\ \Psi_m^{(0)\dagger}(\boldsymbol{r})V_L^{(1)}(\boldsymbol{r})\bar{G}^{(0)}(\boldsymbol{r},\boldsymbol{r}')V_L^{(1)}(\boldsymbol{r}')\Psi_{m'}^{(0)}(\boldsymbol{r}') \quad \left(m,m' = \pm\frac{1}{2},\ L \geqslant 2\right). \tag{B9}$$

Carrying out angular integrations yields

$$\begin{aligned} V_{L,mm'}^{(1,1)} = -\delta_{mm'}\left(\frac{\mu_0}{4\pi}\right)^{-1}\Bigg[&\frac{L}{(2L+1)^2}R_{-L}^{(L,L)}(Q^{(0)},P^{(0)};Q^{(0)},P^{(0)}) \\ &+ \frac{L^2}{(L+1)(2L+1)^2}R_{L+1}^{(L,L)}(Q^{(0)},P^{(0)};Q^{(0)},P^{(0)})\Bigg]\mathbf{D}_L^{(1)}\cdot\mathbf{D}_L^{(1)} \quad \left(m,m' = \pm\frac{1}{2},\ L \geqslant 2\right). \end{aligned} \tag{B10}$$

It is seen that the matrix with elements $V_{L,mm'}^{(1,1)}$ is a multiple of the unit 2×2 matrix. From this, by virtue of Eq. (B8), we infer that the higher-order ($L \geqslant 2$) multipole fields shift the atomic ground state by the quadratic amount

$$E^{(2)} = -\left(\frac{\mu_0}{4\pi}\right)^{-1}\left[\frac{L}{(2L+1)^2}R_{-L}^{(L,L)}(Q^{(0)},P^{(0)};Q^{(0)},P^{(0)}) + \frac{L^2}{(L+1)(2L+1)^2}R_{L+1}^{(L,L)}(Q^{(0)},P^{(0)};Q^{(0)},P^{(0)})\right]\mathbf{D}_L^{(1)}\cdot\mathbf{D}_L^{(1)} \quad (L \geqslant 2), \tag{B11}$$

but do not split it.

It is worthwhile to observe that Eqs. (B7) and (B11) may be united into the one of the form

$$E^{(2)} = -\left(\frac{\mu_0}{4\pi}\right)^{-1}\left[\frac{L}{(2L+1)^2}R_{-L}^{(L,L)}(Q^{(0)},P^{(0)};Q^{(0)},P^{(0)}) + \frac{L^2}{(L+1)(2L+1)^2}R_{L+1}^{(L,L)}(Q^{(0)},P^{(0)};Q^{(0)},P^{(0)})\right]\mathbf{D}_L^{(1)}\cdot\mathbf{D}_L^{(1)} \tag{B12}$$

[notice that Eqs. (B11) and (B12) are *not* identical since in the latter, as opposed to the former, the value of L is not constrained]. Comparison of Eq. (B12) with Eqs. (3.26) and (3.27) reveals the relationship

$$E^{(2)} = -\tfrac{1}{2}\mathbf{M}_L^{(1)}\cdot\mathbf{D}_L^{(1)}. \tag{B13}$$

If the induced-magnetic-moment tensor $\mathbf{M}_L^{(1)}$ is written in the form (3.29), this yields the following expression for the second-order energy correction $E^{(2)}$ in terms of the 2^L-pole magnetizability χ_L:

$$E^{(2)} = -\frac{1}{2}\left(\frac{\mu_0}{4\pi}\right)^{-1}\chi_L\mathbf{D}_L^{(1)}\cdot\mathbf{D}_L^{(1)}. \tag{B14}$$

The reader should compare the relation in Eq. (B14) with its counterpart for the atom immersed in the electric 2^L-pole field, derived by us in Ref. [10, Appendix A].

APPENDIX C: MULTIPOLE CROSS-SUSCEPTIBILITIES VS THE SECOND-ORDER CORRECTION TO THE ATOMIC GROUND-STATE ENERGY IN COMBINED MULTIPOLE ELECTRIC AND MAGNETIC FIELDS

Consider the atom, being initially in its ground state, placed in two superimposed weak fields: an electric one of multipolarity 2^{L_1} and a magnetic one of multipolarity 2^{L_2}, with $L_1 \geqslant 1$ and $L_2 \geqslant 1$. The potential characterizing the interaction of the atomic electron with the resulting field is

$$V_{L_1L_2}^{(1)}(\boldsymbol{r}) = V_{\mathrm{E}L_1}^{(1)}(\boldsymbol{r}) + V_{\mathrm{M}L_2}^{(1)}(\boldsymbol{r}), \tag{C1}$$

where (cf. Ref. [10, Eq. (2.3)])

$$V_{\mathrm{E}L_1}^{(1)}(\boldsymbol{r}) = e\sqrt{\frac{4\pi}{2L_1+1}}\,r^{L_1}\sum_{M_1=-L_1}^{L_1}\mathcal{C}_{L_1M_1}^{(1)*}Y_{L_1M_1}(\boldsymbol{n}_r) \tag{C2}$$

and [cf. Eq. (2.8) of the present work]

$$V^{(1)}_{\mathrm{M}L_2}(\boldsymbol{r}) = -iec\sqrt{\frac{4\pi L_2}{(L_2+1)(2L_2+1)}}\,r^{L_2} \times \sum_{M_2=-L_2}^{L_2} \mathcal{D}^{(1)*}_{L_2M_2}\boldsymbol{\alpha}\cdot\boldsymbol{Y}^{L_2}_{L_2M_2}(\boldsymbol{n}_r). \tag{C3}$$

At first, let us assume that $L_2 \neq 1$. Then it follows from Ref. [10, Sec. II] and from Sec. II of the present work that in the first order of the perturbation theory the interaction (C1) does not affect the energy level in question. Proceeding as in Appendix A, it is easy to show that the second-order energy corrections may be obtained through the diagonalization of the 2×2 matrix $\mathsf{V}^{(1,1)}_{L_1L_2}$ with elements

$$V^{(1,1)}_{L_1L_2,mm'} = -\int_{\mathbb{R}^3} d^3\boldsymbol{r}\int_{\mathbb{R}^3} d^3\boldsymbol{r}'\,\Psi^{(0)\dagger}_m(\boldsymbol{r})V^{(1)}_{L_1L_2}(\boldsymbol{r}) \times \bar{G}^{(0)}(\boldsymbol{r},\boldsymbol{r}')V^{(1)}_{L_1L_2}(\boldsymbol{r}')\Psi^{(0)}_{m'}(\boldsymbol{r}')\quad\left(m,m'=\frac{1}{2}\right), \tag{C4}$$

where the basis spinor functions $\Psi^{(0)}_m(\boldsymbol{r})$ are defined in Eq. (2.15). On carrying out angular integrations, and exploiting the results from Ref. [10, Appendix A] as well as those from Sec. II and from Appendix B of the present work, one deduces that the diagonal and off-diagonal elements of the matrix $\mathsf{V}^{(1,1)}_{L_1L_2}$ are given by

$$\begin{aligned} V^{(1,1)}_{L_1L_2;\pm1/2,\pm1/2} &= -\frac{1}{2}(4\pi\epsilon_0)\alpha_{L_1}\mathsf{C}^{(1)}_{L_1}\cdot\mathsf{C}^{(1)}_{L_1} - \frac{1}{2}\left(\frac{\mu_0}{4\pi}\right)^{-1} \\ &\quad\times \chi_{L_2}\mathsf{D}^{(1)}_{L_2}\cdot\mathsf{D}^{(1)}_{L_2} \mp (\delta_{L_1,L_2-1}+\delta_{L_1,L_2+1}) \\ &\quad\times (4\pi\epsilon_0)c\alpha_{\mathrm{E}L_1\to\mathrm{M}L_2}\frac{\{\mathsf{C}^{(1)}_{L_1}\otimes\mathsf{D}^{(1)}_{L_2}\}_{10}}{\langle L_1 0; L_2 0|10\rangle} \end{aligned} \tag{C5}$$

and

$$V^{(1,1)}_{L_1L_2;\pm1/2,\mp1/2} = \mp(\delta_{L_1,L_2-1}+\delta_{L_1,L_2+1})(4\pi\epsilon_0)c\alpha_{\mathrm{E}L_1\to\mathrm{M}L_2} \times \frac{\sqrt{2}\{\mathsf{C}^{(1)}_{L_1}\otimes\mathsf{D}^{(1)}_{L_2}\}_{1,\mp1}}{\langle L_1 0; L_2 0|10\rangle}, \tag{C6}$$

respectively (recall that $\alpha_{\mathrm{E}L_1\to\mathrm{M}L_2} = \chi_{\mathrm{M}L_2\to\mathrm{E}L_1}$). Hence, with no difficulty, one finds that the two eigenvalues of the matrix $\mathsf{V}^{(1,1)}_{L_1L_2}$ are

$$\begin{aligned} E^{(2)}_{\pm} &= -\frac{1}{2}(4\pi\epsilon_0)\alpha_{L_1}\mathsf{C}^{(1)}_{L_1}\cdot\mathsf{C}^{(1)}_{L_1} - \frac{1}{2}\left(\frac{\mu_0}{4\pi}\right)^{-1}\chi_{L_2}\mathsf{D}^{(1)}_{L_2}\cdot\mathsf{D}^{(1)}_{L_2} \\ &\quad\pm(\delta_{L_1,L_2-1}+\delta_{L_1,L_2+1})(4\pi\epsilon_0)c|\alpha_{\mathrm{E}L_1\to\mathrm{M}L_2}| \\ &\quad\times\frac{|\{\mathsf{C}^{(1)}_{L_1}\otimes\mathsf{D}^{(1)}_{L_2}\}_1|}{|\langle L_1 0; L_2 0|10\rangle|}\quad(L_2\geqslant 2), \end{aligned} \tag{C7}$$

where

$$|\{\mathsf{C}^{(1)}_{L_1}\otimes\mathsf{D}^{(1)}_{L_2}\}_1| = \sqrt{\{\mathsf{C}^{(1)}_{L_1}\otimes\mathsf{D}^{(1)}_{L_2}\}_1\cdot\{\mathsf{C}^{(1)}_{L_1}\otimes\mathsf{D}^{(1)}_{L_2}\}_1} \tag{C8}$$

is the modulus of the vector $\{\mathsf{C}^{(1)}_{L_1}\otimes\mathsf{D}^{(1)}_{L_2}\}_1$. From Eq. (C7) one sees that if $L_1 \neq L_2 \pm 1$ (with $L_2 \neq 1$), then the superposition of the two fields shifts the atomic ground-state level by the amount

$$\begin{aligned} E^{(2)}_0 &= -\frac{1}{2}(4\pi\epsilon_0)\alpha_{L_1}\mathsf{C}^{(1)}_{L_1}\cdot\mathsf{C}^{(1)}_{L_1} \\ &\quad-\frac{1}{2}\left(\frac{\mu_0}{4\pi}\right)^{-1}\chi_{L_2}\mathsf{D}^{(1)}_{L_2}\cdot\mathsf{D}^{(1)}_{L_2}\quad(L_2\geqslant 2), \end{aligned} \tag{C9}$$

but does not remove its degeneracy. A more interesting phenomenon occurs when $L_1 = L_2 \mp 1$, still with $L_2 \geqslant 2$. Then the initial level shifts and splits simultaneously. The two resulting levels are located symmetrically with respect to the energy $E^{(2)}_0$ given above, the gap between them being

$$\Delta E^{(2)} = 2(4\pi\epsilon_0)c|\alpha_{\mathrm{E}L_1\to\mathrm{M}L_2}| \times\frac{|\{\mathsf{C}^{(1)}_{L_1}\otimes\mathsf{D}^{(1)}_{L_2}\}_1|}{|\langle L_1 0; L_2 0|10\rangle|}\quad(L_1 = L_2\pm 1;\ L_2\geqslant 2). \tag{C10}$$

A different situation occurs when the magnetic field is the dipole one, i.e., for $L_2 = 1$. Then (cf. Ref. [10, Sec. II] and Sec. II of the present work) the atomic ground-state level splits in the first order of the perturbation theory. Each of the two resulting levels is nondegenerate, with their energies being given within the first-order perturbation theory by $E^{(0)} + E^{(1)}_{\pm}$ [cf. Eqs. (2.11) and (2.35)]. Within the second-order theory, the energies are approximated as

$$E \simeq E^{(0)} + E^{(1)}_{\pm} + E^{(2)}_{\pm}, \tag{C11}$$

with

$$E^{(2)}_{\pm} = -\int_{\mathbb{R}^3} d^3\boldsymbol{r}\int_{\mathbb{R}^3} d^3\boldsymbol{r}'\,\Psi^{(0)\dagger}_{\pm}(\boldsymbol{r})V^{(1)}_{L_1L_2}(\boldsymbol{r}) \times\bar{G}^{(0)}(\boldsymbol{r},\boldsymbol{r}')V^{(1)}_{L_1L_2}(\boldsymbol{r}')\Psi^{(0)}_{\pm}(\boldsymbol{r}'), \tag{C12}$$

where $\Psi^{(0)}_{\pm}(\boldsymbol{r})$ are the perturbation-adjusted zeroth-order wave functions with the mixing coefficients displayed in Eq. (2.40). Evaluation of the double integral in Eq. (C12) yields eventually

$$\begin{aligned} E^{(2)}_{\pm} &= -\frac{1}{2}(4\pi\epsilon_0)\alpha_{L_1}\mathsf{C}^{(1)}_{L_1}\cdot\mathsf{C}^{(1)}_{L_1} - \frac{1}{2}\left(\frac{\mu_0}{4\pi}\right)^{-1}\chi_1\mathsf{D}^{(1)}_1\cdot\mathsf{D}^{(1)}_1 \\ &\quad\mp\delta_{L_1,2}\sqrt{\frac{5}{2}}(4\pi\epsilon_0)c\alpha_{\mathrm{E}2\to\mathrm{M}1}\boldsymbol{n}\cdot\left\{\mathsf{C}^{(1)}_2\otimes\mathsf{D}^{(1)}_1\right\}_1, \end{aligned} \tag{C13}$$

where $\boldsymbol{n}$ is the unit vector along the magnetic induction vector $\boldsymbol{\mathcal{B}}^{(1)}_1 = \mathsf{D}^{(1)}_1$. Hence, for $L_2 = 1$, to the second order in the perturbation, the gap between the two resulting energy levels is

$$\begin{aligned} \Delta E^{(1)} + \Delta E^{(2)} &= \tfrac{2}{3}(2\gamma_1+1)\mu_{\mathrm{B}}\left|\mathsf{D}^{(1)}_1\right| - \delta_{L_1,2}\sqrt{10}\,(4\pi\epsilon_0) \\ &\quad\times c\alpha_{\mathrm{E}2\to\mathrm{M}1}\boldsymbol{n}\cdot\left\{\mathsf{C}^{(1)}_2\otimes\mathsf{D}^{(1)}_1\right\}_1. \end{aligned} \tag{C14}$$

[1] R. Szmytkowski, The Dirac-Coulomb Sturmians and the series expansion of the Dirac-Coulomb Green function: Application to the relativistic polarizability of the hydrogen-like atom, J. Phys. B **30**, 825 (1997); **30**, 2747(E) (1997); addendum: arXiv:physics/9902050.

[2] R. Szmytkowski, Dynamic polarizability of the relativistic hydrogenlike atom: Application of the Sturmian expansion of the Dirac-Coulomb Green function, Phys. Rev. A **65**, 012503 (2001).

[3] R. Szmytkowski, Magnetizability of the relativistic hydrogen-like atom: application of the Sturmian expansion of the first-order Dirac-Coulomb Green function, J. Phys. B **35**, 1379 (2002).

[4] R. Szmytkowski and K. Mielewczyk, Gordon decomposition of the static dipole polarizability of the relativistic hydrogen-like atom: application of the Sturmian expansion of the first-order Dirac-Coulomb Green function, J. Phys. B **37**, 3961 (2004).

[5] K. Mielewczyk and R. Szmytkowski, Stark-induced magnetic anapole moment in the ground state of the relativistic hydrogenlike atom: Application of the Sturmian expansion of the generalized Dirac-Coulomb Green function, Phys. Rev. A **73**, 022511 (2006); **73**, 039908(E) (2006).

[6] R. Szmytkowski and P. Stefańska, Comment on "Four-component relativistic theory for NMR parameters: Unified formulation and numerical assessment of different approaches," arXiv:1102.1811.

[7] P. Stefańska and R. Szmytkowski, Electric and magnetic dipole shielding constants for the ground state of the relativistic hydrogen-like atom: Application of the Sturmian expansion of the generalized Dirac-Coulomb Green function, Int. J. Quantum Chem. **112**, 1363 (2012).

[8] R. Szmytkowski and P. Stefańska, 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, Phys. Rev. A **85**, 042502 (2012).

[9] R. Szmytkowski and P. Stefańska, Electric-field-induced magnetic quadrupole moment in the ground state of the relativistic hydrogenlike atom: Application of the Sturmian expansion of the generalized Dirac-Coulomb Green function, Phys. Rev. A **89**, 012501 (2014).

[10] R. Szmytkowski and G. Łukasik, Static electric multipole susceptibilities of the relativistic hydrogenlike atom in the ground state: Application of the Sturmian expansion of the generalized Dirac-Coulomb Green function, Phys. Rev. A **93**, 062502 (2016).

[11] R. Szmytkowski and G. Łukasik, Static electric and magnetic multipole susceptibilities for Dirac one-electron atoms in the ground state, At. Data Nucl. Data Tables **111-112**, 41 (2016).

[12] P. Stefańska, Magnetizability of the relativistic hydrogenlike atom in an arbitrary discrete energy eigenstate: Application of the Sturmian expansion of the generalized Dirac-Coulomb Green function, Phys. Rev. A **92**, 032504 (2015).

[13] P. Stefańska, Magnetizabilities of relativistic hydrogenlike atoms in some arbitrary discrete energy eigenstates, At. Data Nucl. Data Tables **108**, 193 (2016).

[14] P. Stefańska, Magnetic-field-induced electric quadrupole moments for relativistic hydrogenlike atoms: Application of the Sturmian expansion of the generalized Dirac-Coulomb Green function, Phys. Rev. A **93**, 022504 (2016).

[15] P. Stefańska, Closed-form expression for the magnetic shielding constant of the relativistic hydrogenlike atom in an arbitrary discrete energy eigenstate: Application of the Sturmian expansion of the generalized Dirac-Coulomb Green function, Phys. Rev. A **94**, 012508 (2016).

[16] P. Stefańska, Magnetic-dipole-to-electric-quadrupole cross-susceptibilities for relativistic hydrogenlike atoms in some low-lying discrete energy eigenstates, At. Data Nucl. Data Tables **113**, 316 (2017).

[17] P. Stefańska, Nuclear magnetic shielding constants of Dirac one-electron atoms in some low-lying discrete energy eigenstates, At. Data Nucl. Data Tables **120**, 352 (2018).

[18] N. L. Manakov, L. P. Rapoport, and S. A. Zapryagaev, Relativistic electromagnetic susceptibilities of hydrogen-like atoms, J. Phys. B **7**, 1076 (1974).

[19] S. A. Zapryagaev, N. L. Manakov, and L. P. Rapoport, Multipole screening of nuclei of hydrogen-like atoms, Yad. Fiz. **19**, 1136 (1974) [English translation: Sov. J. Nucl. Phys. **19**, 582 (1974)].

[20] S. A. Zapryagaev, N. L. Manakov, and V. G. Pal'chikov, *Theory of Multi-charged Ions with One and Two Electrons* (Energoatomizdat, Moscow, 1985) (in Russian), Secs. 4.5 and 4.6.

[21] D. A. Varshalovich, A. N. Moskalev, and V. K. Khersonskii, *Quantum Theory of Angular Momentum* (Nauka, Leningrad, 1975) (in Russian).

[22] R. Szmytkowski, Recurrence and differential relations for spherical spinors, J. Math. Chem. **42**, 397 (2007).

[23] W. Magnus, F. Oberhettinger, and R. P. Soni, *Formulas and Theorems for the Special Functions of Mathematical Physics*, 3rd ed. (Springer, Berlin, 1966).

[24] S. A. Zapryagaev and N. L. Manakov, Application of the Green's function for the Dirac equation to study of relativistic and correlation effects in multicharged ions, Izv. Akad. Nauk SSSR Ser. Fiz. **45**, 2336 (1981).

[25] I. S. Gradshteyn and I. M. Ryzhik, *Table of Integrals, Series, and Products*, 7th ed. (Elsevier, Amsterdam, 2007).

[26] Ya. I. Granovskii and V. I. Nechet, Static effects in hydrogenlike atoms (relativistic theory), Yad. Fiz. **19**, 1290 (1974) [English translation: Sov. J. Nucl. Phys. **19**, 660 (1974)].

[27] L. N. Labzowsky, G. L. Klimchitskaya, and Yu. Yu. Dmitriev, *Relativistic Effects in the Spectra of Atomic Systems* (Institute of Physics, Bristol, 1993), Sec. 6.2.2.

[28] V. G. Pal'chikov and V. P. Shevelko, *Reference Data on Multi-charged Ions* (Springer, Berlin, 1995), Secs. 2.2.4a and 2.4.5a.

[29] P. J. Mohr, D. B. Newell, and B. N. Taylor, CODATA recommended values of the fundamental physical constants: 2014, Rev. Mod. Phys. **88**, 035009 (2016); J. Phys. Chem. Ref. Data **45**, 043102 (2016).

[30] A. Rutkowski and R. Kozłowski, Double perturbation approach to the relativistic hydrogenic atom in a static and uniform magnetic field, J. Phys. B **30**, 1437 (1997).

[31] N. C. Pyper and Z. C. Zhang, Relativistic theory of nuclear shielding in one-electron atoms: 2. Analytical and numerical results, Mol. Phys. **97**, 391 (1999).

[32] E. A. Moore, Relativistic chemical shielding: formally exact solutions for one-electron atoms of maximum total angular momentum for any principal quantum number, Mol. Phys. **97**, 375 (1999).