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

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The ground state of the Dirac one-electron atom, placed in a weak, static electric field of definite 2^L polarity, is studied within the framework of the first-order perturbation theory. The Sturmian expansion of the generalized Dirac-Coulomb Green function [R. Szmytkowski, J. Phys. B: At. Mol. Opt. Phys. **30**, 825 (1997); erratum **30**, 2747 (1997)] is used to derive closed-form analytical expressions for various far-field and near-nucleus static electric multipole susceptibilities of the atom. The far-field multipole susceptibilities—the polarizabilities α_L, the electric-to-magnetic cross susceptibilities $\alpha_{\mathrm{E}L\to\mathrm{M}(L\mp1)}$, and the electric-to-toroidal-magnetic cross susceptibilities $\alpha_{\mathrm{E}L\to\mathrm{T}L}$—are found to be expressible in terms of one or two nonterminating generalized hypergeometric functions ${}_3F_2$ with the unit argument. Counterpart formulas for the near-nucleus multipole susceptibilities—the electric nuclear shielding constants $\sigma_{\mathrm{E}L\to\mathrm{E}L}$, the near-nucleus electric-to-magnetic cross susceptibilities $\sigma_{\mathrm{E}L\to\mathrm{M}(L\mp1)}$, and the near-nucleus electric-to-toroidal-magnetic cross susceptibilities $\sigma_{\mathrm{E}L\to\mathrm{T}L}$—involve one or two terminating ${}_3F_2(1)$ series and for each L may be rewritten in terms of elementary functions. Numerical values of the far-field dipole, quadrupole, octupole, and hexadecapole susceptibilities are provided for selected hydrogenic ions. The effect of a declared uncertainty in the CODATA 2014 recommended value of the fine-structure constant α on the accuracy of numerical results is investigated. Analytical quasirelativistic approximations, valid to the second order in αZ, where Z is the nuclear charge number, are also derived for all types of the far-field and near-nucleus susceptibilities considered in the paper.

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I. INTRODUCTION

Relativistic studies on static multipole polarizabilities of a one-electron atom in its ground state, based on the formalism of the Dirac equation, may be traced back to the early 1970s, when Zon *et al.* [1] presented a closed-form analytical expression for the dipole polarizability α_1 of such a system. The formula given in Ref. [1] involved a particular generalized hypergeometric function ${}_3F_2$ with the unit argument. In the following decades, several equivalent expressions for α_1 were derived, with the use of various alternative analytical techniques, by Labzowsky [2,3], Shestakov and Khristenko [4], Labzowsky *et al.* [5], Le Anh Thu *et al.* [6], Szmytkowski [7], Yakhontov [8], and Szmytkowski and Mielewczyk [9]. Quasirelativistic approximations to α_1, correct to the second order in αZ, where α is the fine-structure constant and Z is the nuclear charge number, were provided by Bartlett and Power [10], Rutkowski and Schwarz [11], and Turski and Sadlej [12] (in this connection, see also the work of Baluja [13]).

In 1974, Manakov *et al.* published a paper [14] (cf. also the review [15] and the monograph [16]) in which they provided an exact analytical formula for a general static multipole polarizability α_L; the formula involved altogether eight different ${}_3F_2(1)$ functions. In the particular case of $L = 1$, the result arrived at in that work might be simplified and the expression from Ref. [1] was recovered. An approximate quasirelativistic representation for α_L, given by Kaneko in Ref. [17] and by Drachman in an erratum to Ref. [18], coincided with the corresponding limit deduced in Ref. [14].[1]

In addition to the analytical works listed above, we have tracked down four papers in which results of purely numerical relativistic calculations of the multipole polarizabilities were reported for selected hydrogenic ions. Goldman [19] carried out variational calculations of the dipole polarizability α_1, employing the Slater-type functions used as a variational basis set. Zhang *et al.* [20] presented results for the quadrupole polarizability α_2 computed with the use of the B-spline Galerkin method. The latter study was pushed further in Ref. [21], where numerical data for α_L with $1 \leqslant L \leqslant 4$ were provided. Finally, very recently Filippin *et al.* [22] applied their Lagrange-mesh method in computations of α_L, with L in the same range as mentioned above. The calculations reported in Refs. [20–22] used the same value of the fine structure constant (taken from the CODATA 2010 recommendation). Numerical data for the four multipole polarizabilities presented by both groups, although obtained with different methods, appeared to be in a very good agreement.

The multipole polarizabilities α_L are closely related to the far-field *electric* multipole moments induced in an atom by external weak, static, electric multipole fields. However, a perturbing electric field may also induce in the atom two kinds of the far-field *magnetic* multipole moments: the plain magnetic moments and the toroidal magnetic moments. Magnitudes of these induced moments may be characterized, respectively, by the so-called electric-to-magnetic and

[1]It should be mentioned that a quasirelativistic expression for α_2 given in Ref. [12] is incorrect and that the criticism of the work [14] presented in an appendix to Ref. [12] is mostly unjustified.

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electric-to-toroidal-magnetic multipole cross susceptibilities. In Ref. [23], Szmytkowski and Stefańska derived an exact closed-form analytical expression for the electric-dipole-to-magnetic-quadrupole cross susceptibility $\alpha_{\mathrm{E}1\to\mathrm{M}2}$ for the Dirac one-electron atom in the ground state. In turn, analytical expressions for the atomic ground-state electric-dipole-to-toroidal-magnetic-dipole cross susceptibility $\alpha_{\mathrm{E}1\to\mathrm{T}1}$ may be inferred from the papers of Lewis and Blinder [24] and Mielewczyk and Szmytkowski [25]. Calculations carried out in Ref. [24] were partly approximate, while those reported in Ref. [25] were exact at the Dirac-Coulomb level.

The three sets of the electric multipole susceptibilities mentioned above characterize, through the moments they are linked to, the first-order field-induced corrections to electromagnetic scalar and vector potentials generated by the atom in the region distant from its nucleus. In analogy, one may consider counterpart susceptibilities related to multipole moments characterizing the first-order corrections to the scalar and vector potentials in the close vicinity of the atomic nucleus. The only fully relativistic research in that direction that we are aware of was done by Zapryagaev *et al.* [26] (cf. also Refs. [15,16]), who studied the electric multipole shielding constants $\sigma_{\mathrm{E}L\to\mathrm{E}L}$. From an exact analytical expression they derived (its explicit, and quite complicated, form was given only in the chronologically latest Ref. [16, Sec. 4.6]), the quasirelativistic estimates for the shielding constants with $L=2$ and $L=3$ were deduced [16,26]. Moreover, a quasirelativistic formula for $\sigma_{\mathrm{E}L\to\mathrm{E}L}$ applicable for any L was derived, in an entirely different way, by Kaneko [17].

This brief state-of-the-art overview of research on electric multipole susceptibilities of the Dirac one-electron atom in the ground state shows that exact analytical expressions for the far- and near-field electric-to-magnetic and electric-to-toroidal-magnetic multipole cross susceptibilities are still missing. We derive them in the present paper, with the aid of an analytical technique based on the Sturmian series representation of the Dirac-Coulomb Green function found by one of us in Ref. [7]. That technique proved its effectiveness in calculations of various properties of hydrogenic ions carried out by our group over the past two decades [9,23,25,27–34]. Moreover, in view of the annoying complexity of the representations for the multipole polarizabilities and the electric shielding constants presented in Refs. [14,16], we have decided to reconsider these two families of atomic susceptibilities, with the goal to arrive at simpler expressions for them. The attempt has appeared to be successful, and below we present formulas for α_L and $\sigma_{\mathrm{E}L\to\mathrm{E}L}$, each one containing only *two* (as opposed to *eight* in Refs. [14,16]) generalized hypergeometric functions ${}_3F_2(1)$.

The structure of the paper is as follows. Section II provides some basic notions and facts concerning the ground state of the Dirac one-electron atom placed in a 2^L-pole electric field. In Secs. III–V, we analyze three kinds of the far-field multipole moments that characterize charge and current distributions of the atom in such a field. We show that if the field is weak, it induces in the atom the electric and toroidal magnetic moments of rank L only, as well as the plain magnetic moments of ranks $L-1$ and $L+1$ (except for the case $L=1$, when only the quadrupole magnetic moment arises). The knowledge of expressions for the induced moments allows one to deduce closed-form formulas for related atomic susceptibilities, and this is subsequently done in each of these sections. We provide exact and approximate (quasirelativistic) expressions for the multipole susceptibilities (the polarizabilities, the electric-to-magnetic cross susceptibilities and the electric-to-toroidal-magnetic cross susceptibilities) and also tabulate their numerical values computed from the exact formulas for selected values of the nuclear charge Z. The effect of a declared uncertainty in the CODATA 2014 [35] recommended value of the inverse of the fine-structure constant on the computed values of the susceptibilities is investigated. Analogous considerations concerning the near-field moments and the susceptibilities related to them are carried out in Secs. VI–VIII. The final Sec. IX contains a brief summary of the most important results derived in the paper, and also discloses our research plans for the near future. The text is supplemented by five appendixes. A relationship between a multipole polarizability and the second-order correction to energy of the atom in a multipole electric field is revealed in Appendix A. In Appendix B, we show how the far- and near-field toroidal magnetic multipole moments arise when the magnetic vector potential is expanded into multipoles. In Appendixes C and D, we prove that for each of the two sets of the toroidal multipole moments that have arisen in Appendix B there is a one-parameter family of equivalent integral expressions, which may be used as their definitions; this gives one the precious freedom to define these moments in forms most suitable for each particular problem in which they emerge. Some properties of the generalized hypergeometric function ${}_3F_2$ with the unit argument, relevant to the material presented in Secs. VI–VIII, are discussed in Appendix E.

II. PRELIMINARIES

Consider a Dirac one-electron atom with a motionless, pointlike, and spinless nucleus of charge $+Ze$. A position vector of the atomic electron relative to the nucleus will be hereafter denoted as $\boldsymbol{r}$. The atom, assumed to be initially in its ground state of energy $E^{(0)}$ [cf. Eq. (2.6)], is perturbed by a static electric 2^L-pole field $\boldsymbol{\mathcal{E}}_L^{(1)}(\boldsymbol{r})$ derivable through the relation $\boldsymbol{\mathcal{E}}_L^{(1)}(\boldsymbol{r}) = -\nabla\varphi_L^{(1)}(\boldsymbol{r})$ from the scalar potential

$$\varphi_L^{(1)}(\boldsymbol{r}) = -\sqrt{\frac{4\pi}{2L+1}}\, r^L \mathsf{C}_L^{(1)} \cdot \mathsf{Y}_L(\boldsymbol{n}_r) \quad (L \geqslant 1), \tag{2.1}$$

where $\mathsf{C}_L^{(1)}$ and $\mathsf{Y}_L(\boldsymbol{n}_r)$ are spherical tensor operators of rank L with components $\mathcal{C}_{LM}^{(1)}$ and $Y_{LM}(\boldsymbol{n}_r)$, respectively. Here $Y_{LM}(\boldsymbol{n}_r)$ is the normalized complex spherical harmonic (in this work, we adopt the Condon-Shortley phase convention) and $\boldsymbol{n}_r$ is the unit vector along $\boldsymbol{r}$. The components of $\mathsf{C}_L^{(1)}$, which determine both the strength of the potential and its angular dependence, are constrained to obey

$$\mathcal{C}_{LM}^{(1)*} = (-)^M \mathcal{C}_{L,-M}^{(1)}, \tag{2.2}$$

where the asterisk denotes the complex conjugation.[2] This ensures that $\varphi_L^{(1)}(\boldsymbol{r})$ is real. In terms of components of the two

[2]The reader should observe that for $L=1$ the components $\mathcal{C}_{1M}^{(1)}$ of the tensor (then vector) $\mathsf{C}_1^{(1)}$ are simply the cyclic components of the perturbing dipole electric field $\boldsymbol{\mathcal{E}}_1^{(1)}$.

tensors, the interaction energy between the atomic electron and the field reads

$$V_L^{(1)}(\boldsymbol{r})=e\sqrt{\frac{4\pi}{2L+1}}\,r^L\sum_{M=-L}^{L}\mathcal{C}_{LM}^{(1)*}Y_{LM}(\boldsymbol{n}_r)\quad(L\geqslant 1).\quad(2.3)$$

Henceforth, it will be assumed that the electric force $-\nabla V_L^{(1)}(\boldsymbol{r})$ acting on the electron is so weak that the probability that the field ionizes the atom may be neglected. Within this approximation, the atomic electron may be considered to be in a stationary state described by the time-independent Dirac equation

$$\left[-ic\hbar\boldsymbol{\alpha}\cdot\nabla+\beta m_e c^2-\frac{Ze^2}{(4\pi\epsilon_0)r}+V_L^{(1)}(\boldsymbol{r})-E\right]\Psi(\boldsymbol{r})=0,\quad(2.4)$$

where $\boldsymbol{\alpha}$ and β are the standard Dirac matrices. Since, by the above-made assumption, the external electric field is weak, in what follows the electron-multipole field interaction term $V_L^{(1)}(\boldsymbol{r})$ is considered as a small perturbation of the Dirac-Coulomb Hamiltonian. Then, to the first order in that perturbation, the energy eigenvalue is

$$E\simeq E^{(0)}+E^{(1)},\quad(2.5)$$

with the (doubly degenerate) unperturbed ground-state energy level $E^{(0)}$ given by

$$E^{(0)}=m_e c^2\gamma_1,\quad(2.6)$$

where

$$\gamma_\kappa=\sqrt{\kappa^2-(\alpha Z)^2}\quad(2.7)$$

(α, not to be confused with the Dirac matrix $\boldsymbol{\alpha}$ or the multipole polarizability α_L, is the Sommerfeld fine-structure constant). To the same order, the electron wave function is

$$\Psi(\boldsymbol{r})\simeq\Psi^{(0)}(\boldsymbol{r})+\Psi^{(1)}(\boldsymbol{r}),\quad(2.8)$$

with the unperturbed component given by

$$\Psi^{(0)}(\boldsymbol{r})=a_{1/2}\Psi_{1/2}^{(0)}(\boldsymbol{r})+a_{-1/2}\Psi_{-1/2}^{(0)}(\boldsymbol{r}).\quad(2.9)$$

The basis states $\Psi_m^{(0)}(\boldsymbol{r})$ appearing in Eq. (2.9) are chosen to be

$$\Psi_m^{(0)}(\boldsymbol{r})=\frac{1}{r}\begin{pmatrix}P^{(0)}(r)\Omega_{-1m}(\boldsymbol{n}_r)\\ iQ^{(0)}(r)\Omega_{1m}(\boldsymbol{n}_r)\end{pmatrix}\quad\left(m=\pm\frac{1}{2}\right),\quad(2.10)$$

where

$$P^{(0)}(r)=-\sqrt{\frac{Z}{a_0}\frac{1+\gamma_1}{\Gamma(2\gamma_1+1)}}\left(\frac{2Zr}{a_0}\right)^{\gamma_1}e^{-Zr/a_0},\quad(2.11\text{a})$$

$$Q^{(0)}(r)=\sqrt{\frac{Z}{a_0}\frac{1-\gamma_1}{\Gamma(2\gamma_1+1)}}\left(\frac{2Zr}{a_0}\right)^{\gamma_1}e^{-Zr/a_0},\quad(2.11\text{b})$$

while $\Omega_{\kappa m_\kappa}(\boldsymbol{n}_r)$ are the spherical spinors [36]. It is easy to verify that the functions (2.10) are orthonormal in the sense of

$$\int_{\mathbb{R}^3}d^3\boldsymbol{r}\,\Psi_m^{(0)\dagger}(\boldsymbol{r})\Psi_{m'}^{(0)}(\boldsymbol{r})=\delta_{mm'}\quad\left(m,m'=\pm\frac{1}{2}\right),\quad(2.12)$$

so that if the coefficients $a_{\pm 1/2}$ are subjected to the constraint

$$|a_{1/2}|^2+|a_{-1/2}|^2=1,\quad(2.13)$$

the function $\Psi^{(0)}(\boldsymbol{r})$ is normalized to unity:

$$\int_{\mathbb{R}^3}d^3\boldsymbol{r}\,\Psi^{(0)\dagger}(\boldsymbol{r})\Psi^{(0)}(\boldsymbol{r})=1.\quad(2.14)$$

It follows from the standard Schrödinger-Rayleigh perturbation theory that the so-far-unknown corrections $E^{(1)}$ and $\Psi^{(1)}(\boldsymbol{r})$ [and also the coefficients $a_{\pm 1/2}$ hidden in $\Psi^{(0)}(\boldsymbol{r})$] enter the inhomogeneous Dirac-Coulomb equation

$$\left[-ic\hbar\boldsymbol{\alpha}\cdot\nabla+\beta m_e c^2-\frac{Ze^2}{(4\pi\epsilon_0)r}-E^{(0)}\right]\Psi^{(1)}(\boldsymbol{r})=-\left[V_L^{(1)}(\boldsymbol{r})-E^{(1)}\right]\Psi^{(0)}(\boldsymbol{r}),\quad(2.15)$$

which is to be solved subject to the usual physical regularity requirements as well as the orthogonality constraints

$$\int_{\mathbb{R}^3}d^3\boldsymbol{r}\,\Psi_m^{(0)\dagger}(\boldsymbol{r})\Psi^{(1)}(\boldsymbol{r})=0\quad\left(m=\pm\frac{1}{2}\right).\quad(2.16)$$

After Eq. (2.15) is projected onto the unperturbed basis states $\Psi_m^{(0)}(\boldsymbol{r})$, ($m=\pm\frac{1}{2}$), this yields the homogeneous algebraic system

$$\sum_{m'=-1/2}^{1/2}\left[V_{L,mm'}^{(1)}-E^{(1)}\delta_{mm'}\right]a_{m'}=0\quad\left(m=\pm\frac{1}{2}\right),\quad(2.17)$$

where

$$V_{L,mm'}^{(1)}=e\sqrt{\frac{4\pi}{2L+1}}\sum_{M=-L}^{L}\mathcal{C}_{LM}^{(1)*}\times\int_{\mathbb{R}^3}d^3\boldsymbol{r}\,\Psi_m^{(0)\dagger}(\boldsymbol{r})r^L Y_{LM}(\boldsymbol{n}_r)\Psi_{m'}^{(0)}(\boldsymbol{r}).\quad(2.18)$$

Denoting

$$\langle\Omega_{\kappa m_\kappa}|Y_{LM}\Omega_{\kappa' m_{\kappa'}}\rangle\equiv\oint_{4\pi}d^2\boldsymbol{n}_r\,\Omega_{\kappa m_\kappa}^{\dagger}(\boldsymbol{n}_r)Y_{LM}(\boldsymbol{n}_r)\Omega_{\kappa' m_{\kappa'}}(\boldsymbol{n}_r)\quad(2.19)$$

and exploiting the known identity

$$\langle\Omega_{-\kappa m_\kappa}|Y_{\lambda\mu}\Omega_{-\kappa' m_{\kappa'}}\rangle=\langle\Omega_{\kappa m_\kappa}|Y_{\lambda\mu}\Omega_{\kappa' m_{\kappa'}}\rangle,\quad(2.20)$$

we obtain

$$V_{L,mm'}^{(1)}=e\sqrt{\frac{4\pi}{2L+1}}\int_0^\infty dr\,r^L\{[P^{(0)}(r)]^2+[Q^{(0)}(r)]^2\}\times\sum_{M=-L}^{L}\mathcal{C}_{LM}^{(1)*}\langle\Omega_{-1m}|Y_{LM}\Omega_{-1m'}\rangle.\quad(2.21)$$

The angular integral in Eq. (2.21) may be evaluated with the aid of the known formula

$$\sqrt{\frac{4\pi}{2L+1}}\langle\Omega_{\kappa m_\kappa}|Y_{LM}\Omega_{\kappa' m_{\kappa'}}\rangle = (-)^{m_\kappa+1/2}2\sqrt{|\kappa\kappa'|}\begin{pmatrix}|\kappa|-\frac{1}{2} & L & |\kappa'|-\frac{1}{2}\\ -\frac{1}{2} & 0 & \frac{1}{2}\end{pmatrix} \times\begin{pmatrix}|\kappa|-\frac{1}{2} & L & |\kappa'|-\frac{1}{2}\\ m_\kappa & -M & -m_{\kappa'}\end{pmatrix}\Pi(l_\kappa,L,l_{\kappa'}), \quad (2.22)$$

where $\left(\begin{smallmatrix}j_a & j_b & j_c\\ m_a & m_b & m_c\end{smallmatrix}\right)$ denotes Wigner's $3j$ coefficient, while

$$\Pi(l_\kappa,L,l_{\kappa'}) = \begin{cases}1 & \text{for } l_\kappa+L+l_{\kappa'} \text{ even},\\ 0 & \text{for } l_\kappa+L+l_{\kappa'} \text{ odd},\end{cases} \quad (2.23)$$

with

$$l_\kappa = \left|\kappa+\tfrac{1}{2}\right|-\tfrac{1}{2} \quad (2.24)$$

and similarly for $l_{\kappa'}$. One finds

$$\langle\Omega_{-1m}|Y_{LM}\Omega_{-1m'}\rangle = \frac{1}{\sqrt{4\pi}}\delta_{L0}\delta_{M0}\delta_{mm'}. \quad (2.25)$$

Since we have excluded the case $L=0$ from the very beginning, we have

$$V^{(1)}_{L,mm'} = 0, \quad (2.26)$$

which implies immediately [cf. Eq. (2.17)] that for any L it holds that

$$E^{(1)} = 0 \quad (2.27)$$

and that the coefficients $a_{\pm 1/2}$ are arbitrary save for the normalization condition (2.13).

With the result (2.27) in mind, the solution to Eq. (2.15) may be written as

$$\Psi^{(1)}(\boldsymbol{r}) = -e\sqrt{\frac{4\pi}{2L+1}}\sum_{M=-L}^{L}\mathcal{C}^{(1)*}_{LM} \times\int_{\mathbb{R}^3}d^3\boldsymbol{r}'\bar{G}^{(0)}(\boldsymbol{r},\boldsymbol{r}')r'^L Y_{LM}(\boldsymbol{n}'_r)\Psi^{(0)}(\boldsymbol{r}'), \quad (2.28)$$

where $\bar{G}^{(0)}(\boldsymbol{r},\boldsymbol{r}')$ is the generalized (or reduced) Dirac-Coulomb Green function [7, Sec. 6] associated with the ground state of the atom under investigation.

III. ELECTRIC MULTIPOLE MOMENTS OF THE ATOM IN THE MULTIPOLE ELECTRIC FIELD AND ATOMIC MULTIPOLE POLARIZABILITIES

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

Being in the state described by the wave function $\Psi(\boldsymbol{r})$, the electronic cloud of the atom may be characterized, among others, by its electric multipole moments Q_λ with the spherical components[3]

$$\mathcal{Q}_{\lambda\mu} = \sqrt{\frac{4\pi}{2\lambda+1}}\int_{\mathbb{R}^3}d^3\boldsymbol{r}\,r^\lambda Y_{\lambda\mu}(\boldsymbol{n}_r)\rho(\boldsymbol{r}), \quad (3.1)$$

where

$$\rho(\boldsymbol{r}) = \frac{-e\Psi^\dagger(\boldsymbol{r})\Psi(\boldsymbol{r})}{\int_{\mathbb{R}^3}d^3\boldsymbol{r}'\Psi^\dagger(\boldsymbol{r}')\Psi(\boldsymbol{r}')} \quad (3.2)$$

may be considered as a smeared electronic charge density. In the case the function $\Psi(\boldsymbol{r})$ may be approximated as in Eq. (2.8), after Eqs. (2.9), (2.14), and (2.16) are taken into account, the density $\rho(\boldsymbol{r})$ may be approximately written as

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

where

$$\rho^{(0)}(\boldsymbol{r}) = -e\Psi^{(0)\dagger}(\boldsymbol{r})\Psi^{(0)}(\boldsymbol{r}) \quad (3.4)$$

and

$$\rho^{(1)}(\boldsymbol{r}) = -2e\,\mathrm{Re}[\Psi^{(0)\dagger}(\boldsymbol{r})\Psi^{(1)}(\boldsymbol{r})]. \quad (3.5)$$

Accordingly, Eq. (3.3) implies

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

where

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

and

$$\mathcal{Q}^{(1)}_{\lambda\mu} = -e\sqrt{\frac{4\pi}{2\lambda+1}}\int_{\mathbb{R}^3}d^3\boldsymbol{r}\,r^\lambda Y_{\lambda\mu}(\boldsymbol{n}_r)[\Psi^{(0)\dagger}(\boldsymbol{r})\Psi^{(1)}(\boldsymbol{r}) + \Psi^{(1)\dagger}(\boldsymbol{r})\Psi^{(0)}(\boldsymbol{r})] \quad (3.8)$$

are the permanent and the first-order induced electric multipole moments of the electronic cloud, respectively. Proceeding along the route that parallels the evaluation of the energy correction $E^{(1)}$, presented in Sec. II, it is easy to show that the only nonvanishing multipole moment of the atom in the unperturbed ground state is the monopole one:

$$\mathcal{Q}^{(0)}_{\lambda\mu} = \mathcal{Q}^{(0)}_{\lambda\mu}\delta_{\lambda 0}\delta_{\mu 0}, \quad \mathcal{Q}^{(0)}_{00} = -e. \quad (3.9)$$

Therefore, in what follows we shall be concerned with the evaluation of the induced moment $\mathcal{Q}^{(1)}_{\lambda\mu}$ only.

With the aid of the identity

$$Y_{\lambda\mu}(\boldsymbol{n}_r) = (-)^\mu Y^*_{\lambda,-\mu}(\boldsymbol{n}_r) \quad (3.10)$$

and of the result in Eq. (2.28), $\mathcal{Q}^{(1)}_{\lambda\mu}$ may be written as

$$\mathcal{Q}^{(1)}_{\lambda\mu} = \tilde{\mathcal{Q}}^{(1)}_{\lambda\mu} + (-)^\mu\tilde{\mathcal{Q}}^{(1)*}_{\lambda,-\mu}, \quad (3.11)$$

[3]The reader should observe that the definition (3.1) of the spherical components of the electric multipole moments we adopt here differs from the one we used in Ref. [31] in that in the latter the spherical harmonic was complex conjugated.

with

$$\widetilde{\mathcal{Q}}_{\lambda\mu}^{(1)} = e^2 \frac{4\pi}{\sqrt{(2\lambda+1)(2L+1)}} \sum_{M=-L}^{L} \mathcal{C}_{LM}^{(1)*} \int_{\mathbb{R}^3} d^3\boldsymbol{r} \int_{\mathbb{R}^3} d^3\boldsymbol{r}' \Psi^{(0)\dagger}(\boldsymbol{r}) r^{\lambda} Y_{\lambda\mu}(\boldsymbol{n}_r) \bar{G}^{(0)}(\boldsymbol{r},\boldsymbol{r}') r'^{L} Y_{LM}(\boldsymbol{n}'_r) \Psi^{(0)}(\boldsymbol{r}'). \tag{3.12}$$

It is possible to separate out radial and angular integrations in Eq. (3.12). To this end, one may exploit the following multipole expansion of the generalized Green function $\bar{G}^{(0)}(\boldsymbol{r},\boldsymbol{r}')$:

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

After this expansion is plugged into Eq. (3.12) and use is made of Eq. (2.20), one arrives at

$$\widetilde{\mathcal{Q}}_{\lambda\mu}^{(1)} = (4\pi\epsilon_0) \frac{4\pi}{\sqrt{(2\lambda+1)(2L+1)}} \sum_{\substack{\kappa=-\infty \\ (\kappa\neq 0)}}^{\infty} R_{\kappa}^{(\lambda,L)}(P^{(0)},Q^{(0)};P^{(0)},Q^{(0)})$$

$$\times \sum_{M=-L}^{L} \sum_{m_\kappa=-|\kappa|+1/2}^{|\kappa|-1/2} \sum_{m=-1/2}^{1/2} \sum_{m'=-1/2}^{1/2} a_m^* a_{m'} \mathcal{C}_{LM}^{(1)*} \langle \Omega_{-1m} | Y_{\lambda\mu} \Omega_{\kappa m_\kappa} \rangle \langle \Omega_{\kappa m_\kappa} | Y_{LM} \Omega_{-1m'} \rangle, \tag{3.14}$$

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

$$R_{\kappa}^{(L_1,L_2)}(F_a,F_b;F_c,F_d) = \int_0^\infty dr \int_0^\infty dr' (F_a(r) \quad F_b(r)) r^{L_1} \bar{\mathsf{G}}_{\kappa}^{(0)}(r,r') r'^{L_2} \begin{pmatrix} F_c(r') \\ F_d(r') \end{pmatrix} \tag{3.15}$$

(other particular forms of this integral will appear in Secs. IV to VIII), with the matrix

$$\bar{\mathsf{G}}_{\kappa}^{(0)}(r,r') = \begin{pmatrix} \bar{g}_{(++)\kappa}^{(0)}(r,r') & \bar{g}_{(+-)\kappa}^{(0)}(r,r') \\ \bar{g}_{(-+)\kappa}^{(0)}(r,r') & \bar{g}_{(--)\kappa}^{(0)}(r,r') \end{pmatrix} \tag{3.16}$$

being the radial generalized Dirac-Coulomb Green function associated with the ground-state atomic energy level (2.6). The two angular integrals in Eq. (3.14) may be taken with the help of the general formula (2.22). Once this is done, it is then possible to carry out summations over the quantum numbers m_κ, m, and m'. After straightforward, though tedious, calculations, one finds that the only nonvanishing contributions to $\widetilde{\mathcal{Q}}_{\lambda\mu}^{(1)}$ come from the terms with $\kappa = L$ and $\kappa = -L-1$; one has

$$\widetilde{\mathcal{Q}}_{\lambda\mu}^{(1)} = \widetilde{\mathcal{Q}}_{\lambda\mu,L}^{(1)} + \widetilde{\mathcal{Q}}_{\lambda\mu,-L-1}^{(1)}, \tag{3.17}$$

with

$$\widetilde{\mathcal{Q}}_{\lambda\mu,\kappa}^{(1)} = \delta_{\lambda L}(4\pi\epsilon_0) \frac{\mathrm{sgn}(\kappa)}{(2L+1)^2} R_{\kappa}^{(L,L)}(P^{(0)},Q^{(0)};P^{(0)},Q^{(0)}) \big\{ [\kappa + \mu(|a_{1/2}|^2 - |a_{-1/2}|^2)] \mathcal{C}_{L\mu}^{(1)}$$

$$+ \sqrt{(L-\mu)(L+\mu+1)}\, a_{1/2} a_{-1/2}^* \mathcal{C}_{L,\mu+1}^{(1)} + \sqrt{(L+\mu)(L-\mu+1)}\, a_{1/2}^* a_{-1/2} \mathcal{C}_{L,\mu-1}^{(1)} \big\} \quad (\kappa = L, -L-1). \tag{3.18}$$

The asterisks at the components of the tensor $\mathsf{C}_L^{(1)}$ in the above equation have disappeared in virtue of the identity (2.2). With Eqs. (3.17) and (3.18) in hand, we return back to Eq. (3.11). This eventually yields $\mathcal{Q}_{\lambda\mu}^{(1)}$ in the form

$$\mathcal{Q}_{\lambda\mu}^{(1)} = \mathcal{Q}_{\lambda\mu}^{(1)} \delta_{\lambda L}, \tag{3.19}$$

with

$$\mathcal{Q}_{L\mu}^{(1)} = \mathcal{Q}_{L\mu,L}^{(1)} + \mathcal{Q}_{L\mu,-L-1}^{(1)}, \tag{3.20}$$

where

$$\mathcal{Q}_{L\mu,\kappa}^{(1)} = (4\pi\epsilon_0) \frac{2|\kappa|}{(2L+1)^2} R_{\kappa}^{(L,L)}(P^{(0)},Q^{(0)};P^{(0)},Q^{(0)}) \mathcal{C}_{L\mu}^{(1)} \quad (\kappa = L, -L-1). \tag{3.21}$$

Equation (3.19) shows that the only electric moment induced in the atom is that one which is precisely of the same multipole character as the perturbing electric field. In other words, one has

$$\mathsf{Q}_\lambda \simeq \mathsf{Q}_\lambda^{(0)} \delta_{\lambda 0} + \mathsf{Q}_\lambda^{(1)} \delta_{\lambda L}. \tag{3.22}$$

B. Atomic multipole polarizabilities

The 2^L-pole polarizability of the atom in the ground state, $\alpha_{\mathrm{E}L\to\mathrm{E}L}$, is defined as a proportionality factor between the induced electric multipole moment $\mathsf{Q}_L^{(1)}$ and the field tensor $\mathsf{C}_L^{(1)}$ appearing in the expression (2.1) for the perturbing 2^L-pole electric potential:[4]

$$\mathsf{Q}_L^{(1)} = (4\pi\epsilon_0)\alpha_{\mathrm{E}L\to\mathrm{E}L}\mathsf{C}_L^{(1)} \tag{3.23}$$

(the SI factor $4\pi\epsilon_0$ has been separated out in order to secure that the physical dimension of $\alpha_{\mathrm{E}L\to\mathrm{E}L}$ is L^{2L+1}, where L stands for length). It follows from Eqs. (3.23) and (3.20)–(3.22) that the polarizability $\alpha_{\mathrm{E}L\to\mathrm{E}L}$, hereafter denoted in the standard manner as α_L, may be written as the sum

$$\alpha_L = \alpha_{L,L} + \alpha_{L,-L-1}, \tag{3.24}$$

with the constituents being given by

$$\alpha_{L,\kappa} = \frac{2|\kappa|}{(2L+1)^2} R_\kappa^{(L,L)}(P^{(0)},Q^{(0)};P^{(0)},Q^{(0)}) \qquad (\kappa = L, -L-1). \tag{3.25}$$

The remaining task is to evaluate the double radial integral $R_\kappa^{(L,L)}(P^{(0)},Q^{(0)};P^{(0)},Q^{(0)})$. This will be done below with the aid of the Sturmian expansion of the radial generalized Dirac-Coulomb Green function [7]:

$$\bar{\mathsf{G}}_\kappa^{(0)}(r,r') = \sum_{n_r=-\infty}^{\infty} \frac{1}{\mu_{n_r\kappa}^{(0)} - 1} \begin{pmatrix} S_{n_r\kappa}^{(0)}(r) \\ T_{n_r\kappa}^{(0)}(r) \end{pmatrix} \begin{pmatrix} \mu_{n_r\kappa}^{(0)} S_{n_r\kappa}^{(0)}(r') & T_{n_r\kappa}^{(0)}(r') \end{pmatrix} \quad (\kappa \neq -1), \tag{3.26}$$

where

$$S_{n_r\kappa}^{(0)}(r) = \sqrt{\frac{(1+\gamma_1)(|n_r|+2\gamma_\kappa)|n_r|!}{2ZN_{n_r\kappa}(N_{n_r\kappa}-\kappa)\Gamma(|n_r|+2\gamma_\kappa)}} \left(\frac{2Zr}{a_0}\right)^{\gamma_\kappa} e^{-Zr/a_0} \left[L_{|n_r|-1}^{(2\gamma_\kappa)}\left(\frac{2Zr}{a_0}\right) + \frac{\kappa - N_{n_r\kappa}}{|n_r|+2\gamma_\kappa} L_{|n_r|}^{(2\gamma_\kappa)}\left(\frac{2Zr}{a_0}\right)\right] \tag{3.27a}$$

and

$$T_{n_r\kappa}^{(0)}(r) = \sqrt{\frac{(1-\gamma_1)(|n_r|+2\gamma_\kappa)|n_r|!}{2ZN_{n_r\kappa}(N_{n_r\kappa}-\kappa)\Gamma(|n_r|+2\gamma_\kappa)}} \left(\frac{2Zr}{a_0}\right)^{\gamma_\kappa} e^{-Zr/a_0} \left[L_{|n_r|-1}^{(2\gamma_\kappa)}\left(\frac{2Zr}{a_0}\right) - \frac{\kappa - N_{n_r\kappa}}{|n_r|+2\gamma_\kappa} L_{|n_r|}^{(2\gamma_\kappa)}\left(\frac{2Zr}{a_0}\right)\right] \tag{3.27b}$$

are the radial Dirac-Coulomb Sturmian functions associated with the atomic ground-state energy level (2.6) [here $L_n^{(\alpha)}(\rho)$ denotes the generalized Laguerre polynomial [37]; we define $L_{-1}^{(\alpha)}(\rho) \equiv 0$], while

$$\mu_{n_r\kappa}^{(0)} = \frac{|n_r| + \gamma_\kappa + N_{n_r\kappa}}{\gamma_1 + 1} \tag{3.28}$$

is the pertinent Sturmian eigenvalue. The "apparent principal quantum number" appearing in Eqs. (3.27) and (3.28) is defined as

$$N_{n_r\kappa} = \pm\sqrt{(|n_r| + \gamma_\kappa)^2 + (\alpha Z)^2} = \pm\sqrt{|n_r|^2 + 2|n_r|\gamma_\kappa + \kappa^2}, \tag{3.29}$$

where the plus sign is to be chosen for $n_r > 0$ and the minus sign for $n_r < 0$; for $n_r = 0$ one should choose the plus sign if $\kappa < 0$ and the minus sign if $\kappa > 0$, i.e., one has $N_{0\kappa} = -\kappa$.

Substitution of the expansion (3.26) into the definition of the double radial integral which appears in Eq. (3.25) yields $\alpha_{L,\kappa}$ in the form

$$\alpha_{L,\kappa} = \frac{2|\kappa|}{(2L+1)^2} \sum_{n_r=-\infty}^{\infty} \frac{1}{\mu_{n_r\kappa}^{(0)} - 1} \int_0^\infty dr\, r^L \left[P^{(0)}(r)S_{n_r\kappa}^{(0)}(r) + Q^{(0)}(r)T_{n_r\kappa}^{(0)}(r)\right] \times \int_0^\infty dr'\, r'^L \left[\mu_{n_r\kappa}^{(0)} P^{(0)}(r')S_{n_r\kappa}^{(0)}(r') + Q^{(0)}(r')T_{n_r\kappa}^{(0)}(r')\right] \quad (\kappa = L, -L-1). \tag{3.30}$$

The evident advantage of the use of the Sturmian expansion (3.26) is that in the resulting Eq. (3.30) the integrations over r and r' may be carried out separately. On exploiting Eqs. (2.11), (3.27), and (3.28), the integral formula [38, Eq. (7.414.11)]

$$\int_0^\infty d\rho\, \rho^\gamma e^{-\rho} L_n^{(\alpha)}(\rho) = \frac{\Gamma(\gamma+1)\Gamma(n+\alpha-\gamma)}{n!\Gamma(\alpha-\gamma)} \quad (\mathrm{Re}\,\gamma > -1) \tag{3.31}$$

and the identity

$$\gamma_\kappa^2 = \gamma_1^2 + \kappa^2 - 1, \tag{3.32}$$

[4]The multipole polarizability $\alpha_{EL\to EL}$ may be equivalently defined through the formula $E^{(2)} = -\frac{1}{2}(4\pi\epsilon_0)\alpha_{\mathrm{E}L\to\mathrm{E}L}\mathsf{C}_L^{(1)}\cdot\mathsf{C}_L^{(1)}$, where $E^{(2)}$ is the second-order correction to energy. The reader is referred to Appendix A for the justification of this statement.

one finds that

$$\int_0^\infty dr r^L\big[P^{(0)}(r)S^{(0)}_{n_r\kappa}(r)+Q^{(0)}(r)T^{(0)}_{n_r\kappa}(r)\big]$$
$$=-\left(\frac{a_0}{2Z}\right)^{L+1}\frac{\sqrt{2}(N_{n_r\kappa}-\kappa)[\gamma_1(N_{n_r\kappa}+\kappa)-(|n_r|+\gamma_\kappa-\gamma_1-L-1)]}{\sqrt{a_0|n_r|!N_{n_r\kappa}(N_{n_r\kappa}-\kappa)\Gamma(2\gamma_1+1)\Gamma(|n_r|+2\gamma_\kappa+1)}}\frac{\Gamma(\gamma_\kappa+\gamma_1+L+1)\Gamma(|n_r|+\gamma_\kappa-\gamma_1-L-1)}{\Gamma(\gamma_\kappa-\gamma_1-L)} \tag{3.33}$$

and

$$\int_0^\infty dr r^L\big[\mu^{(0)}_{n_r\kappa}P^{(0)}(r)S^{(0)}_{n_r\kappa}(r)+Q^{(0)}(r)T^{(0)}_{n_r\kappa}(r)\big]$$
$$=-\left(\frac{a_0}{2Z}\right)^{L+1}\frac{\big(\mu^{(0)}_{n_r\kappa}-1\big)(N_{n_r\kappa}-\kappa)}{\sqrt{2a_0|n_r|!N_{n_r\kappa}(N_{n_r\kappa}-\kappa)\Gamma(2\gamma_1+1)\Gamma(|n_r|+2\gamma_\kappa+1)}}\frac{\Gamma(\gamma_\kappa+\gamma_1+L+1)\Gamma(|n_r|+\gamma_\kappa-\gamma_1-L-1)}{\Gamma(\gamma_\kappa-\gamma_1-L)}$$
$$\times\left\{[(N_{n_r\kappa}+\kappa)-\gamma_1(|n_r|+\gamma_\kappa-\gamma_1-L-1)]+\frac{N_{n_r\kappa}+1}{|n_r|+\gamma_\kappa-\gamma_1}[\gamma_1(N_{n_r\kappa}+\kappa)-(|n_r|+\gamma_\kappa-\gamma_1-L-1)]\right\}. \tag{3.34}$$

Once these two equations are plugged into Eq. (3.30), then use is made of Eqs. (3.29) and (3.32) and subsequently the terms in the summand corresponding to the same absolute value of the summation index n_r are collected together, with a good deal of labor one finds the following infinite-series representation for $\alpha_{L,\kappa}$:

$$\alpha_{L,\kappa}=\frac{a_0^{2L+1}}{Z^{2L+2}}\frac{|\kappa|\Gamma^2(\gamma_\kappa+\gamma_1+L+1)}{2^{2L}(2L+1)^2\Gamma(2\gamma_1+1)\Gamma^2(\gamma_\kappa-\gamma_1-L)}\left\{\gamma_1[\gamma_1(\kappa+1)+2(L+1)]\sum_{n_r=0}^{\infty}\frac{\Gamma^2(n_r+\gamma_\kappa-\gamma_1-L)}{n_r!(n_r+\gamma_\kappa-\gamma_1+1)\Gamma(n_r+2\gamma_\kappa+1)}\right.$$
$$\left.-(\kappa-1)\sum_{n_r=0}^{\infty}\frac{\Gamma^2(n_r+\gamma_\kappa-\gamma_1-L)}{n_r!(n_r+\gamma_\kappa-\gamma_1)\Gamma(n_r+2\gamma_\kappa+1)}\right\}\quad(\kappa=L,-L-1). \tag{3.35}$$

The two series in Eq. (3.35) may be expressed in terms of the generalized hypergeometric function ${}_3F_2$ of the unit argument. With the aid of the identity

$$\sum_{n=0}^{\infty}\frac{\Gamma(n+a_1)\Gamma(n+a_2)\Gamma(n+a_3)}{n!\Gamma(n+b_1)\Gamma(n+b_2)}=\frac{\Gamma(a_1)\Gamma(a_2)\Gamma(a_3)}{\Gamma(b_1)\Gamma(b_2)}\,{}_3F_2\left(\begin{matrix}a_1,a_2,a_3\\ b_1,b_2\end{matrix};1\right)\quad[\mathrm{Re}(b_1+b_2-a_1-a_2-a_3)>0], \tag{3.36}$$

one arrives at

$$\alpha_{L,\kappa}=\frac{a_0^{2L+1}}{Z^{2L+2}}\frac{|\kappa|\Gamma^2(\gamma_\kappa+\gamma_1+L+1)}{2^{2L}(2L+1)^2\Gamma(2\gamma_1+1)\Gamma(2\gamma_\kappa+1)}$$
$$\times\left\{\frac{\gamma_1[\gamma_1(\kappa+1)+2(L+1)]}{\gamma_\kappa-\gamma_1+1}\,{}_3F_2\left(\begin{matrix}\gamma_\kappa-\gamma_1-L,\ \gamma_\kappa-\gamma_1-L,\ \gamma_\kappa-\gamma_1+1\\ \gamma_\kappa-\gamma_1+2,\ 2\gamma_\kappa+1\end{matrix};1\right)\right.$$
$$\left.-\frac{\gamma_\kappa+\gamma_1}{\kappa+1}\,{}_3F_2\left(\begin{matrix}\gamma_\kappa-\gamma_1-L,\ \gamma_\kappa-\gamma_1-L,\ \gamma_\kappa-\gamma_1\\ \gamma_\kappa-\gamma_1+1,\ 2\gamma_\kappa+1\end{matrix};1\right)\right\}\quad(\kappa=L,-L-1). \tag{3.37}$$

A simplification of the above result may be attained with the help of the relation

$${}_3F_2\left(\begin{matrix}a_1,a_2,a_3\\ a_3+1,b\end{matrix};1\right)=\frac{\Gamma(b)\Gamma(b-a_1-a_2+1)}{(b-a_3-1)\Gamma(b-a_1)\Gamma(b-a_2)}-\frac{(a_1-a_3-1)(a_2-a_3-1)}{(a_3+1)(b-a_3-1)}\,{}_3F_2\left(\begin{matrix}a_1,a_2,a_3+1\\ a_3+2,b\end{matrix};1\right)$$
$$[\mathrm{Re}(b-a_1-a_2)>-1], \tag{3.38}$$

which may be used to eliminate one of the two ${}_3F_2(1)$'s in favor of the other. It appears that a bit more compact result is obtained if the first ${}_3F_2(1)$ is retained:

$$\alpha_{L,\kappa}=\frac{a_0^{2L+1}}{Z^{2L+2}}\frac{|\kappa|\Gamma(2\gamma_1+2L+2)}{2^{2L}(\kappa+1)(2L+1)^2\Gamma(2\gamma_1+1)}\left\{-1+\frac{[\gamma_1(\kappa+1)+L+1]^2\Gamma^2(\gamma_\kappa+\gamma_1+L+1)}{(\gamma_\kappa-\gamma_1+1)\Gamma(2\gamma_1+2L+2)\Gamma(2\gamma_\kappa+1)}\right.$$
$$\left.\times\,{}_3F_2\left(\begin{matrix}\gamma_\kappa-\gamma_1-L,\ \gamma_\kappa-\gamma_1-L,\ \gamma_\kappa-\gamma_1+1\\ \gamma_\kappa-\gamma_1+2,\ 2\gamma_\kappa+1\end{matrix};1\right)\right\}\quad(\kappa=L,-L-1). \tag{3.39}$$

Specializing to the two admitted values of κ, we finally arrive at

$$\alpha_{L,L} = \frac{a_0^{2L+1}}{Z^{2L+2}} \frac{L\Gamma(2\gamma_1+2L+2)}{2^{2L}(L+1)(2L+1)^2\Gamma(2\gamma_1+1)}\bigg\{-1 + \frac{(L+1)^2(\gamma_1+1)^2\Gamma^2(\gamma_L+\gamma_1+L+1)}{(\gamma_L-\gamma_1+1)\Gamma(2\gamma_1+2L+2)\Gamma(2\gamma_L+1)} \times {}_3F_2\left(\begin{matrix}\gamma_L-\gamma_1-L,\ \gamma_L-\gamma_1-L,\ \gamma_L-\gamma_1+1\\ \gamma_L-\gamma_1+2,\ 2\gamma_L+1\end{matrix};1\right)\bigg\} \tag{3.40a}$$

and

$$\alpha_{L,-L-1} = \frac{a_0^{2L+1}}{Z^{2L+2}} \frac{(L+1)\Gamma(2\gamma_1+2L+2)}{2^{2L}L(2L+1)^2\Gamma(2\gamma_1+1)}\bigg\{1 - \frac{(L\gamma_1-L-1)^2\Gamma^2(\gamma_{L+1}+\gamma_1+L+1)}{(\gamma_{L+1}-\gamma_1+1)\Gamma(2\gamma_1+2L+2)\Gamma(2\gamma_{L+1}+1)} \times {}_3F_2\left(\begin{matrix}\gamma_{L+1}-\gamma_1-L,\ \gamma_{L+1}-\gamma_1-L,\ \gamma_{L+1}-\gamma_1+1\\ \gamma_{L+1}-\gamma_1+2,\ 2\gamma_{L+1}+1\end{matrix};1\right)\bigg\}, \tag{3.40b}$$

respectively. Hence, the closed-form expression for the 2^L-pole polarizability of the hydrogenlike in the ground state is

$$\alpha_L = \frac{a_0^{2L+1}}{Z^{2L+2}} \frac{\Gamma(2\gamma_1+2L+2)}{2^{2L}L(L+1)(2L+1)\Gamma(2\gamma_1+1)}\bigg\{1 + \frac{L^2(L+1)^2(\gamma_1+1)^2\Gamma^2(\gamma_L+\gamma_1+L+1)}{(2L+1)(\gamma_L-\gamma_1+1)\Gamma(2\gamma_1+2L+2)\Gamma(2\gamma_L+1)} \times {}_3F_2\left(\begin{matrix}\gamma_L-\gamma_1-L,\ \gamma_L-\gamma_1-L,\ \gamma_L-\gamma_1+1\\ \gamma_L-\gamma_1+2,\ 2\gamma_L+1\end{matrix};1\right) - \frac{(L+1)^2(L\gamma_1-L-1)^2\Gamma^2(\gamma_{L+1}+\gamma_1+L+1)}{(2L+1)(\gamma_{L+1}-\gamma_1+1)\Gamma(2\gamma_1+2L+2)\Gamma(2\gamma_{L+1}+1)} \times {}_3F_2\left(\begin{matrix}\gamma_{L+1}-\gamma_1-L,\ \gamma_{L+1}-\gamma_1-L,\ \gamma_{L+1}-\gamma_1+1\\ \gamma_{L+1}-\gamma_1+2,\ 2\gamma_{L+1}+1\end{matrix};1\right)\bigg\}. \tag{3.41}$$

In the dipole case ($L = 1$), Eq. (3.41) yields

$$\alpha_1 = \frac{a_0^3}{Z^4}\bigg\{\frac{(\gamma_1+1)(2\gamma_1+1)(4\gamma_1^2+13\gamma_1+12)}{36} - \frac{(\gamma_1-2)^2\Gamma^2(\gamma_2+\gamma_1+2)}{18(\gamma_2-\gamma_1+1)\Gamma(2\gamma_1+1)\Gamma(2\gamma_2+1)} \times {}_3F_2\left(\begin{matrix}\gamma_2-\gamma_1-1,\ \gamma_2-\gamma_1-1,\ \gamma_2-\gamma_1+1\\ \gamma_2-\gamma_1+2,\ 2\gamma_2+1\end{matrix};1\right)\bigg\}, \tag{3.42}$$

which is in agreement with earlier findings (cf. Refs. [8, Eq. (16)] and [9, Eq. (3.24)]).

Exact numerical values of the dipole to hexadecapole polarizabilities for the ground state of the hydrogen ($Z = 1$) atom, derived directly from the analytical formula (3.41), are presented in Table I. Calculations have been done for two values of the inverse of the fine-structure constant: $\alpha^{-1} = 137.035\,999\,139$ (from CODATA 2014 [35]) and $\alpha^{-1} = 137.035\,999\,074$ (from CODATA 2010 [39]), in the latter case with the purpose to enable one to make comparison with data available in Refs. [21,22]. Table I confirms almost perfect numerical accuracy of results obtained computationally by Tang *et al.* [21] using the B-spline Galerkin method and also the high quality of numbers generated by Filippin *et al.* [22] with the use of the Langrange-mesh method. Actually, one encounters essentially the same situation for ions with higher atomic numbers Z: Our data (not provided here) generated from Eq. (3.41) with the CODATA 2010 value of α^{-1} validate completely counterpart numbers from Refs. [20,21] and imply only minor inaccuracies (the maximal relative error being of the order of 10^{-12}) in the data listed in Ref. [22].

It should be stressed that both sets of our data presented in Table I, as well as the numbers excerpted for comparison from Refs. [20–22], have been computed under the assumption that the values of the inverse of the fine structure constant used in calculations are exact numbers. Actually, available values of α^{-1} are always subject to experimental uncertainties. In particular, the CODATA 2014 recommended value of α^{-1} appears to be $137.035\,999\,139\,(31)$, where the number in parentheses is a one-standard-deviation uncertainty in the last two digits of the significand [35]. It is evident that this uncertainty implies limitations on physically meaningful numbers of digits in values of computed quantities and has an impact on uncertainties in digits to be retained. In Table II, we present results of our numerical calculations of the first four multipole polarizabilities α_L for selected hydrogenic ions with the nuclear charge numbers from the range $1 \leqslant Z \leqslant 137$. Computations have again been based on the use of the formula displayed in Eq. (3.41), but now the uncertainty in the value of α^{-1} has been taken into account. The values of the polarizabilities are listed along with uncertainties in their last two digits.

In the final step, we provide an approximate formula for the polarizability α_L that is correct to the second order in αZ. Using

$$\gamma_\kappa \simeq |\kappa| - \frac{(\alpha Z)^2}{2|\kappa|} \tag{3.43}$$

and

$$\Gamma(a\gamma_\kappa + a'\gamma_{\kappa'} + b) \simeq \Gamma(a|\kappa| + a'|\kappa'| + b)\bigg[1 - \frac{(\alpha Z)^2}{2}\left(\frac{a}{|\kappa|} + \frac{a'}{|\kappa'|}\right) \times \psi(a|\kappa| + a'|\kappa'| + b)\bigg], \tag{3.44}$$

TABLE I. Comparison of present exact values of the static electric dipole, quadrupole, octupole, and hexadecapole polarizabilities for the hydrogen atom ($Z = 1$) in the ground state with those obtained numerically by other authors using either the *B*-spline Galerkin method [21] or the Lagrange-mesh method [22]. The present results have been computed from the analytical formula in Eq. (3.41), using both the currently recommended CODATA 2014 value of the inverse of the fine-structure constant α^{-1} and, for the sake of making comparison with the results from Refs. [21,22] more explicit, also its previous CODATA 2010 value.

Source	α_1 (units of a_0^3)	α_2 (units of a_0^5)	α_3 (units of a_0^7)	α_4 (units of a_0^9)
		$\alpha^{-1} = 137.035\,999\,139$ (from CODATA 2014)		
Present (exact)	4.499 751 495 177 875 011 523 552	1.499 882 982 285 755 177 470 692 × 10^1	1.312 378 214 478 562 151 040 415 × 10^2	2.126 028 674 499 338 786 454 128 × 10^3
		$\alpha^{-1} = 137.035\,999\,074$ (from CODATA 2010)		
Present (exact)	4.499 751 495 177 639 267 396 013	1.499 882 982 285 644 169 960 840 × 10^1	1.312 378 214 478 446 621 510 730 × 10^2	2.126 028 674 499 128 831 459 952 × 10^3
Ref. [21]	4.499 751 495 177 639 267 396 02	1.499 882 982 285 644 169 960 8 × 10^1	1.312 378 214 478 446 621 510 × 10^2	2.126 028 674 499 128 831 46 × 10^3
Ref. [22]	4.499 751 495 177 639	1.499 882 982 285 648 × 10^1	1.312 378 214 478 460 × 10^2	2.126 028 674 499 147 × 10^3

where

$$\psi(z) = \frac{1}{\Gamma(z)}\frac{d\Gamma(z)}{dz} \tag{3.45}$$

is the digamma function, one finds

$$ {}_3F_2\left(\begin{matrix}\gamma_L-\gamma_1-L,\ \gamma_L-\gamma_1-L,\ \gamma_L-\gamma_1+1\\ \gamma_L-\gamma_1+2,\ 2\gamma_L+1\end{matrix};1\right) \simeq \frac{2L^2+4L+1}{(L+1)(2L+1)} - (\alpha Z)^2\frac{4L^4+2L^3-8L^2-3L+1}{2L(L+1)^2(2L+1)^2} \tag{3.46}$$

and

$$ {}_3F_2\left(\begin{matrix}\gamma_{L+1}-\gamma_1-L,\ \gamma_{L+1}-\gamma_1-L,\ \gamma_{L+1}-\gamma_1+1\\ \gamma_{L+1}-\gamma_1+2,\ 2\gamma_{L+1}+1\end{matrix};1\right) \simeq 1, \tag{3.47}$$

and, further,

$$\alpha_{L,L} \simeq \frac{a_0^{2L+1}}{Z^{2L+2}}\frac{(L+2)(2L)!}{2^{2L}} \times\left\{1-(\alpha Z)^2\left[\psi(2L+3)-\psi(3) + \frac{2L^5+7L^4+6L^3-L-1}{L^2(L+1)(L+2)(2L+1)}\right]\right\}, \tag{3.48a}$$

$$\alpha_{L,-L-1} \simeq \frac{a_0^{2L+1}}{Z^{2L+2}}\frac{(L+1)(L+2)(2L-1)!}{2^{2L-1}} \times\left\{1-(\alpha Z)^2\left[\psi(2L+3)-\psi(3) + \frac{4L^3+10L^2+7L+2}{2(L+1)^2(L+2)(2L+1)}\right]\right\}. \tag{3.48b}$$

Adding Eqs. (3.48a) and (3.48b) yields an approximation to α_L,

$$\alpha_L \simeq \frac{a_0^{2L+1}}{Z^{2L+2}}\frac{(L+2)(2L+1)!}{2^{2L}L} \times\left\{1-(\alpha Z)^2\left[\psi(2L+3)-\psi(3) + \frac{4L^5+18L^4+22L^3+7L^2-2}{2L(L+1)(L+2)(2L+1)^2}\right]\right\}, \tag{3.49}$$

which is identical to the one given in Refs. [14–16] and may be also shown to be equivalent to the counterpart expressions given in Ref. [17] and in an erratum to Ref. [18]. If in the above equation one uses recursively the relation

$$\psi(z+1) = \psi(z) + \frac{1}{z}, \tag{3.50}$$

a bit more compact approximation to α_L is obtained:

$$\alpha_L \simeq \frac{a_0^{2L+1}}{Z^{2L+2}}\frac{(L+2)(2L+1)!}{2^{2L}L}\left\{1-(\alpha Z)^2\left[\psi(2L)-\psi(2) + \frac{14L^3+43L^2+40L+15}{2(L+1)(L+2)(2L+1)^2}\right]\right\}. \tag{3.51}$$

TABLE II. The static electric multipole polarizabilities α_L with $1 \leqslant L \leqslant 4$ for selected hydrogenic ions in the ground state, computed from the analytical formula in Eq. (3.41). 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	α_1 (units of a_0^3)	α_2 (units of a_0^5)	α_3 (units of a_0^7)	α_4 (units of a_0^9)
1	4.499 751 495 177 88 (12)	1.499 882 982 285 755 (53) $\times 10^{1}$	1.312 378 214 478 562 (55) $\times 10^{2}$	2.126 028 674 499 34 (10) $\times 10^{3}$
2	2.811 878 749 185 62 (28) $\times 10^{-1}$	2.343 018 679 358 61 (34) $\times 10^{-1}$	5.125 050 375 239 51 (86) $\times 10^{-1}$	2.075 551 546 062 03 (40)
5	7.190 061 246 057 0 (45) $\times 10^{-3}$	9.581 285 372 341 8 (85) $\times 10^{-4}$	3.352 210 608 794 4 (35) $\times 10^{-4}$	2.171 618 426 950 9 (26) $\times 10^{-4}$
10	4.475 164 360 649 (11) $\times 10^{-4}$	1.488 319 383 924 5 (53) $\times 10^{-5}$	1.300 352 899 799 1 (55) $\times 10^{-6}$	2.104 187 645 771 (10) $\times 10^{-7}$
20	2.750 523 499 121 (28) $\times 10^{-5}$	2.271 146 583 119 (33) $\times 10^{-7}$	4.938 640 072 446 (84) $\times 10^{-9}$	1.991 062 443 097 (38) $\times 10^{-10}$
40	1.604 002 839 693 (69) $\times 10^{-6}$	3.218 326 876 78 (20) $\times 10^{-9}$	1.717 671 116 98 (12) $\times 10^{-11}$	1.707 067 336 75 (14) $\times 10^{-13}$
60	2.797 090 475 04 (30) $\times 10^{-7}$	2.371 147 053 79 (36) $\times 10^{-10}$	5.443 579 082 03 (97) $\times 10^{-13}$	2.345 208 225 06 (47) $\times 10^{-15}$
80	7.256 230 367 0 (16) $\times 10^{-8}$	3.196 013 750 5 (10) $\times 10^{-11}$	3.921 694 890 3 (15) $\times 10^{-14}$	9.141 669 900 2 (38) $\times 10^{-17}$
100	2.168 647 589 56 (99) $\times 10^{-8}$	5.405 559 190 6 (34) $\times 10^{-12}$	3.923 335 160 2 (29) $\times 10^{-15}$	5.514 202 255 9 (46) $\times 10^{-18}$
120	5.962 322 886 3 (66) $\times 10^{-9}$	8.350 889 829 (13) $\times 10^{-13}$	3.675 741 125 2 (65) $\times 10^{-16}$	3.240 357 008 3 (64) $\times 10^{-19}$
137	5.748 648 40 (30) $\times 10^{-10}$	3.159 735 44 (23) $\times 10^{-14}$	6.689 221 53 (60) $\times 10^{-18}$	3.139 717 91 (33) $\times 10^{-21}$

Explicit expressions for the quasirelativistic approximations to α_L with $1 \leqslant L \leqslant 4$, resulting from Eq. (3.51), are displayed in Table III.

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

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

Next we proceed to the investigation of electric-field-induced magnetic multipole moments of the Dirac one-electron atom in the ground state. In Appendix B, components of the 2^L-pole magnetic moment M_λ for a stationary sourceless current distribution $\boldsymbol{j}(\boldsymbol{r})$ are defined as

$$\mathcal{M}_{\lambda\mu} = -i\sqrt{\frac{4\pi\lambda}{(\lambda+1)(2\lambda+1)}}\int_{\mathbb{R}^3} d^3\boldsymbol{r}\, r^\lambda \boldsymbol{Y}^\lambda_{\lambda\mu}(\boldsymbol{n}_r)\cdot\boldsymbol{j}(\boldsymbol{r}), \tag{4.1}$$

where $\boldsymbol{Y}^\lambda_{\lambda\mu}(\boldsymbol{n}_r)$ is a particular vector spherical harmonic [40, Sec. 7.3.1]. The right-hand side of Eq. (4.1) may be transformed to another form using the identity [40, Sec. 7.3.1]

$$\boldsymbol{Y}^\lambda_{\lambda\mu}(\boldsymbol{n}_r) = \frac{\boldsymbol{\Lambda} Y_{\lambda\mu}(\boldsymbol{n}_r)}{\sqrt{\lambda(\lambda+1)}}, \tag{4.2}$$

TABLE III. Quasirelativistic approximations for the static electric multipole polarizabilities α_L with $1 \leqslant L \leqslant 4$ for the Dirac one-electron atom in the ground state. The expressions have been derived from Eq. (3.51).

L	α_L
1	$\frac{a_0^3}{Z^4}\frac{9}{2}\left[1-\frac{28}{27}(\alpha Z)^2\right]$
2	$\frac{a_0^5}{Z^6}15\left[1-\frac{293}{200}(\alpha Z)^2\right]$
3	$\frac{a_0^7}{Z^8}\frac{525}{4}\left[1-\frac{5123}{2940}(\alpha Z)^2\right]$
4	$\frac{a_0^9}{Z^{10}}\frac{8505}{4}\left[1-\frac{33251}{17010}(\alpha Z)^2\right]$

where

$$\boldsymbol{\Lambda} = -i\boldsymbol{r}\times\boldsymbol{\nabla} \tag{4.3}$$

is the orbital angular momentum operator. Plugging Eq. (4.2) into Eq. (4.1), after exploiting the Hermiticity property of the operator $\boldsymbol{\Lambda}$, one obtains the formula

$$\mathcal{M}_{\lambda\mu} = \frac{i}{\lambda+1}\sqrt{\frac{4\pi}{2\lambda+1}}\int_{\mathbb{R}^3} d^3\boldsymbol{r}\, r^\lambda Y_{\lambda\mu}(\boldsymbol{n}_r)\boldsymbol{\Lambda}\cdot\boldsymbol{j}(\boldsymbol{r}), \tag{4.4}$$

which appears to be optimal for the use in the subsequent considerations.

In the weak-perturbing-field case considered in this work, the atomic wave function may be approximated as in Eq. (2.8). Hence, after using Eqs. (2.9), (2.14), and (2.16), to the first order in the perturbing electric multipole field, the electronic current in the atom

$$\boldsymbol{j}(\boldsymbol{r}) = \frac{-ec\Psi^\dagger(\boldsymbol{r})\boldsymbol{\alpha}\Psi(\boldsymbol{r})}{\int_{\mathbb{R}^3} d^3\boldsymbol{r}'\,\Psi^\dagger(\boldsymbol{r}')\Psi(\boldsymbol{r}')} \tag{4.5}$$

may be approximated as

$$\boldsymbol{j}(\boldsymbol{r}) \simeq \boldsymbol{j}^{(0)}(\boldsymbol{r}) + \boldsymbol{j}^{(1)}(\boldsymbol{r}), \tag{4.6}$$

where

$$\boldsymbol{j}^{(0)}(\boldsymbol{r}) = -ec\Psi^{(0)\dagger}(\boldsymbol{r})\boldsymbol{\alpha}\Psi^{(0)}(\boldsymbol{r}) \tag{4.7}$$

is the electronic current in the unperturbed atomic ground state, while

$$\boldsymbol{j}^{(1)}(\boldsymbol{r}) = -2ec\,\mathrm{Re}[\Psi^{(0)\dagger}(\boldsymbol{r})\boldsymbol{\alpha}\Psi^{(1)}(\boldsymbol{r})] \tag{4.8}$$

is the leading term in the field-induced electronic current. The approximation in Eq. (4.6) implies that

$$\mathcal{M}_{\lambda\mu} \simeq \mathcal{M}^{(0)}_{\lambda\mu} + \mathcal{M}^{(1)}_{\lambda\mu}, \tag{4.9}$$

where

$$\mathcal{M}^{(0)}_{\lambda\mu} = \frac{i}{\lambda+1}\sqrt{\frac{4\pi}{2\lambda+1}}\int_{\mathbb{R}^3} d^3\boldsymbol{r}\, r^\lambda Y_{\lambda\mu}(\boldsymbol{n}_r)\boldsymbol{\Lambda}\cdot\boldsymbol{j}^{(0)}(\boldsymbol{r}) \tag{4.10}$$

are components of the magnetic 2^λ-pole moment of the atom in the unperturbed state $\Psi^{(0)}(\boldsymbol{r})$, while

$$\mathcal{M}^{(1)}_{\lambda\mu} = \frac{i}{\lambda+1}\sqrt{\frac{4\pi}{2\lambda+1}}\int_{\mathbb{R}^3} d^3\boldsymbol{r}\, r^\lambda Y_{\lambda\mu}(\boldsymbol{n}_r)\boldsymbol{\Lambda}\cdot\boldsymbol{j}^{(1)}(\boldsymbol{r}) \tag{4.11}$$

is the first-order field-induced correction to $\mathcal{M}^{(0)}_{\lambda\mu}$.

It has been shown by us in Ref. [23] that the only nonvanishing unperturbed multipole moment $\mathsf{M}^{(0)}_\lambda$ is the dipole one,

$$\mathcal{M}^{(0)}_{\lambda\mu} = \mathcal{M}^{(0)}_{\lambda\mu}\delta_{\lambda 1}, \tag{4.12}$$

the spherical components of which are

$$\mathcal{M}^{(0)}_{1,0} = -\frac{1}{3}(2\gamma_1+1)\mu_{\mathrm{B}}(|a_{1/2}|^2 - |a_{-1/2}|^2), \tag{4.13a}$$

$$\mathcal{M}^{(0)}_{1,\pm1} = \pm\frac{\sqrt{2}}{3}(2\gamma_1+1)\mu_{\mathrm{B}} a^*_{\pm1/2}a_{\mp1/2}, \tag{4.13b}$$

where

$$\mu_{\mathrm{B}} = \frac{e\hbar}{2m_e} \tag{4.14}$$

is the Bohr magneton. If we introduce the unit vector $\boldsymbol{\nu}$ with the cyclic components

$$\nu_0 = |a_{1/2}|^2 - |a_{-1/2}|^2, \quad \nu_{\pm1} = \mp\sqrt{2}\, a^*_{\pm1/2}a_{\mp1/2}, \tag{4.15}$$

the magnetic dipole moment vector may be compactly written as

$$\mathsf{M}^{(0)}_1 = -\frac{2\gamma_1+1}{3}\mu_{\mathrm{B}}\boldsymbol{\nu}. \tag{4.16}$$

The parametrization

$$a_{1/2} = e^{-i(\chi+\phi)/2}\cos(\vartheta/2), \quad a_{-1/2} = e^{-i(\chi-\phi)/2}\sin(\vartheta/2)$$
$$(0 \leqslant \chi,\phi < 2\pi,\ 0 \leqslant \vartheta \leqslant \pi) \tag{4.17}$$

implies that

$$\nu_0 = \cos\vartheta, \quad \nu_{\pm1} = \mp\frac{1}{\sqrt{2}}e^{\pm i\phi}\sin\vartheta; \tag{4.18}$$

i.e., ϑ and ϕ may be considered as the polar and the azimuthal angles, respectively, of the vector $\boldsymbol{\nu}$ in the spherical coordinate system.

Once the nature of the unperturbed moments has been explained, we proceed to the analysis of the induced moments $\mathsf{M}^{(1)}_\lambda$. Substituting the expression (4.8) for the induced current into the definition (4.11), after using the identity (3.10), we obtain

$$\mathcal{M}^{(1)}_{\lambda\mu} = \widetilde{\mathcal{M}}^{(1)}_{\lambda\mu} + (-)^\mu\widetilde{\mathcal{M}}^{(1)*}_{\lambda,-\mu}, \tag{4.19}$$

where

$$\widetilde{\mathcal{M}}^{(1)}_{\lambda\mu} = -\frac{iec}{\lambda+1}\sqrt{\frac{4\pi}{2\lambda+1}}\int_{\mathbb{R}^3} d^3\boldsymbol{r}\, r^\lambda Y_{\lambda\mu}(\boldsymbol{n}_r)\boldsymbol{\Lambda} \cdot[\Psi^{(0)\dagger}(\boldsymbol{r})\boldsymbol{\alpha}\Psi^{(1)}(\boldsymbol{r})]. \tag{4.20}$$

As $\Psi^{(1)}(\boldsymbol{r})$ is given by Eq. (2.28), the above equation may be rewritten in the form of the double integral

$$\widetilde{\mathcal{M}}^{(1)}_{\lambda\mu} = \frac{ie^2c}{\lambda+1}\frac{4\pi}{\sqrt{(2\lambda+1)(2L+1)}}\sum_{M=-L}^{L}\mathcal{C}^{(1)*}_{LM} \times\int_{\mathbb{R}^3} d^3\boldsymbol{r}\int_{\mathbb{R}^3} d^3\boldsymbol{r}'\, r^\lambda Y_{\lambda\mu}(\boldsymbol{n}_r)\boldsymbol{\Lambda} \cdot[\Psi^{(0)\dagger}(\boldsymbol{r})\boldsymbol{\alpha}\bar{G}^{(0)}(\boldsymbol{r},\boldsymbol{r}')]r'^L Y_{LM}(\boldsymbol{n}'_r)\Psi^{(0)}(\boldsymbol{r}'). \tag{4.21}$$

A simplification occurs if one exploits the obvious identity

$$\boldsymbol{\Lambda}\cdot[\Psi^{(0)\dagger}(\boldsymbol{r})\boldsymbol{\alpha}\bar{G}^{(0)}(\boldsymbol{r},\boldsymbol{r}')] = -[\boldsymbol{\alpha}\cdot\boldsymbol{\Lambda}\Psi^{(0)}(\boldsymbol{r})]^\dagger\bar{G}^{(0)}(\boldsymbol{r},\boldsymbol{r}') +\Psi^{(0)\dagger}(\boldsymbol{r})\boldsymbol{\alpha}\cdot\boldsymbol{\Lambda}\bar{G}^{(0)}(\boldsymbol{r},\boldsymbol{r}'), \tag{4.22}$$

the multipole expansion (3.13) of the Green function $\bar{G}^{(0)}(\boldsymbol{r},\boldsymbol{r}')$, and the relation [36, Eq. (3.2.3)]

$$\boldsymbol{\sigma}\cdot\boldsymbol{\Lambda}\Omega_{\kappa m_\kappa}(\boldsymbol{n}_r) = -(\kappa+1)\Omega_{\kappa m_\kappa}(\boldsymbol{n}_r). \tag{4.23}$$

This results in a separation of integrations over radial and angular variables, and one obtains

$$\widetilde{\mathcal{M}}^{(1)}_{\lambda\mu} = -\frac{(4\pi\epsilon_0)c}{\lambda+1}\frac{4\pi}{\sqrt{(2\lambda+1)(2L+1)}} \times\sum_{\substack{\kappa=-\infty\\(\kappa\neq0)}}^{\infty}(\kappa-1)R^{(\lambda,L)}_\kappa(Q^{(0)},P^{(0)};P^{(0)},Q^{(0)}) \times\sum_{M=-L}^{L}\sum_{m_\kappa=-|\kappa|+1/2}^{|\kappa|-1/2}\sum_{m=-1/2}^{1/2}\sum_{m'=-1/2}^{1/2}a^*_m a_{m'}\mathcal{C}^{(1)*}_{LM} \times\langle\Omega_{-1m}|Y_{\lambda\mu}\Omega_{-\kappa m_\kappa}\rangle\langle\Omega_{\kappa m_\kappa}|Y_{LM}\Omega_{-1m'}\rangle, \tag{4.24}$$

where $R^{(\lambda,L)}_\kappa(Q^{(0)},P^{(0)};P^{(0)},Q^{(0)})$ is a particular case of the double radial integral defined in Eq. (3.15) and the bracket notation has been used to denote the angular integrals [cf. Eq. (2.19)]. Evaluating the latter with the aid of the formula in Eq. (2.22) and carrying out the summations, we find that $\widetilde{\mathcal{M}}^{(1)}_{\lambda\mu}$ does not vanish only if $\lambda = L\mp1$, i.e.,

$$\widetilde{\mathcal{M}}^{(1)}_{\lambda\mu} = \widetilde{\mathcal{M}}^{(1)}_{\lambda\mu}\delta_{\lambda,L-1} + \widetilde{\mathcal{M}}^{(1)}_{\lambda\mu}\delta_{\lambda,L+1}. \tag{4.25}$$

In these two cases, one has

$$\widetilde{\mathcal{M}}^{(1)}_{L-1,\mu} = -(4\pi\epsilon_0)c\,\frac{L-1}{L(4L^2-1)}R^{(L-1,L)}_L(Q^{(0)},P^{(0)};P^{(0)},Q^{(0)})\big[-\sqrt{L^2-\mu^2}\,(|a_{1/2}|^2-|a_{-1/2}|^2)\mathcal{C}^{(1)}_{L\mu} +\sqrt{(L+\mu)(L+\mu+1)}\,a_{1/2}a^*_{-1/2}\mathcal{C}^{(1)}_{L,\mu+1} - \sqrt{(L-\mu)(L-\mu+1)}\,a^*_{1/2}a_{-1/2}\mathcal{C}^{(1)}_{L,\mu-1}\big] \tag{4.26}$$

and

$$\widetilde{\mathcal{M}}^{(1)}_{L+1,\mu} = -(4\pi\epsilon_0)c\,\frac{1}{(2L+1)(2L+3)}R^{(L+1,L)}_{-L-1}(Q^{(0)},P^{(0)};P^{(0)},Q^{(0)})\big[\sqrt{(L+1)^2-\mu^2}\,(|a_{1/2}|^2-|a_{-1/2}|^2)\mathcal{C}^{(1)}_{L\mu} +\sqrt{(L-\mu)(L-\mu+1)}a_{1/2}a^*_{-1/2}\mathcal{C}^{(1)}_{L,\mu+1} - \sqrt{(L+\mu)(L+\mu+1)}a^*_{1/2}a_{-1/2}\mathcal{C}^{(1)}_{L,\mu-1}\big], \tag{4.27}$$

respectively. On combining Eqs. (4.19), (4.25)–(4.27), and (4.15), we find that

$$\mathcal{M}_{\lambda\mu}^{(1)} = \mathcal{M}_{\lambda\mu}^{(1)}\delta_{\lambda,L-1} + \mathcal{M}_{\lambda\mu}^{(1)}\delta_{\lambda,L+1}, \tag{4.28}$$

where

$$\mathcal{M}_{L-1,\mu}^{(1)} = -(4\pi\epsilon_0)c\,\frac{2(L-1)}{L(4L^2-1)}R_L^{(L-1,L)}(Q^{(0)},P^{(0)};P^{(0)},Q^{(0)})\Big[-\sqrt{L^2-\mu^2}\,\nu_0\mathcal{C}_{L\mu}^{(1)} + \sqrt{\tfrac{1}{2}(L+\mu)(L+\mu+1)}\,\nu_{-1}\mathcal{C}_{L,\mu+1}^{(1)} + \sqrt{\tfrac{1}{2}(L-\mu)(L-\mu+1)}\,\nu_1\mathcal{C}_{L,\mu-1}^{(1)}\Big] \tag{4.29}$$

and

$$\mathcal{M}_{L+1,\mu}^{(1)} = -(4\pi\epsilon_0)c\,\frac{2}{(2L+1)(2L+3)}R_{-L-1}^{(L+1,L)}(Q^{(0)},P^{(0)};P^{(0)},Q^{(0)})\Big[\sqrt{(L+1)^2-\mu^2}\,\nu_0\mathcal{C}_{L\mu}^{(1)} + \sqrt{\tfrac{1}{2}(L-\mu)(L-\mu+1)}\,\nu_{-1}\mathcal{C}_{L,\mu+1}^{(1)} + \sqrt{\tfrac{1}{2}(L+\mu)(L+\mu+1)}\,\nu_1\mathcal{C}_{L,\mu-1}^{(1)}\Big]. \tag{4.30}$$

Thus, we see that, to the first-order of accuracy, the 2^L-pole electric field induces in the ground state of the atom *two* magnetic multipole moments, being the 2^{L-1}-pole and the 2^{L+1}-pole ones; i.e.,

$$\mathsf{M}_\lambda \simeq \mathsf{M}_\lambda^{(0)}\delta_{\lambda 1} + \mathsf{M}_\lambda^{(1)}(\delta_{\lambda,L-1} + \delta_{\lambda,L+1}). \tag{4.31}$$

However, it is evident from Eq. (4.29) that an exception occurs in the case of the perturbing electric dipole ($L = 1$) field, when only the *quadrupole* ($\lambda = 2$) moment is induced (cf. Ref. [23]).

Consider now the irreducible spherical tensor product of rank λ of the vector $\boldsymbol{\nu}$, defined in Eq. (4.15) and characterizing the unperturbed atomic state, and the tensor $\mathsf{C}_L^{(1)}$, characterizing the perturbing multipole electric field. According to the general theory of such products [40, Sec. 3.1.7], its components are given by

$$\{\boldsymbol{\nu}\otimes\mathsf{C}_L^{(1)}\}_{\lambda\mu} = \sum_{m=-1}^{1}\sum_{M=-L}^{L}\langle 1mLM|\lambda\mu\rangle\nu_m\mathcal{C}_{LM}^{(1)}, \tag{4.32}$$

where $\langle 1mLM|\lambda\mu\rangle$ is a particular Clebsch-Gordan coefficient. A look at a table of these coefficients (e.g., Ref. [40, Table 8.2]) shows that the two induced magnetic moments $\mathsf{M}_{L\mp1}^{(1)}$, components of which are displayed in Eqs. (4.29) and (4.30), may be compactly written as

$$\mathsf{M}_\lambda^{(1)} = -(4\pi\epsilon_0)c\,\frac{2\sqrt{2}\,\lambda}{(2\lambda+1)\sqrt{(2L+1)(\lambda+L+1)}}R_{\kappa_\lambda}^{(\lambda,L)}(Q^{(0)},P^{(0)};P^{(0)},Q^{(0)})\{\boldsymbol{\nu}\otimes\mathsf{C}_L^{(1)}\}_\lambda \quad (\lambda = L\mp1), \tag{4.33}$$

with

$$\kappa_\lambda = -\frac{1}{2}(\lambda-L)(\lambda+L+1) = \begin{cases} L & \text{for } \lambda = L-1,\\ -L-1 & \text{for } \lambda = L+1.\end{cases} \tag{4.34}$$

B. Atomic multipole EL → M($L \mp 1$) cross susceptibilities

We define the atomic electric-to-magnetic multipole cross susceptibilities $\alpha_{\mathrm{E}L\to\mathrm{M}(L\mp1)}$ through the relation

$$\mathsf{M}_\lambda^{(1)} = (4\pi\epsilon_0)c\,\alpha_{\mathrm{E}L\to\mathrm{M}\lambda}\frac{\{\boldsymbol{\nu}\otimes\mathsf{C}_L^{(1)}\}_\lambda}{\langle 10L0|\lambda0\rangle} \quad (\lambda = L\mp1), \tag{4.35}$$

where the Clebsch-Gordan coefficient standing in the denominator in the fraction on the right-hand side is

$$\langle 10L0|\lambda0\rangle = (\lambda-L)\sqrt{\frac{\lambda+L+1}{2(2L+1)}} \quad (\lambda = L\mp1). \tag{4.36}$$

Combining Eq. (4.35) with the representation (4.33) of the tensor $\mathsf{M}_\lambda^{(1)}$ links the cross susceptibility to the double radial integral appearing therein:

$$\alpha_{\mathrm{E}L\to\mathrm{M}\lambda} = -\frac{2\lambda(\lambda-L)}{(2\lambda+1)(2L+1)}R_{\kappa_\lambda}^{(\lambda,L)}(Q^{(0)},P^{(0)};P^{(0)},Q^{(0)}) \quad (\lambda = L\mp1). \tag{4.37}$$

To tackle the latter, we exploit the Sturmian expansion (3.26), obtaining

$$\alpha_{\mathrm{EL}\to\mathrm{M}\lambda} = -\frac{2\lambda(\lambda-L)}{(2\lambda+1)(2L+1)}\sum_{n_r=-\infty}^{\infty}\frac{1}{\mu^{(0)}_{n_r\kappa_\lambda}-1}\int_0^\infty dr\, r^{\lambda}\big[Q^{(0)}(r)S^{(0)}_{n_r\kappa_\lambda}(r)+P^{(0)}(r)T^{(0)}_{n_r\kappa_\lambda}(r)\big]$$
$$\times\int_0^\infty dr'\, r'^{L}\big[\mu^{(0)}_{n_r\kappa_\lambda}P^{(0)}(r')S^{(0)}_{n_r\kappa_\lambda}(r')+Q^{(0)}(r')T^{(0)}_{n_r\kappa_\lambda}(r')\big]\quad(\lambda=L\mp1). \tag{4.38}$$

The second of the two, now separated, radial integrals in Eq. (4.38) is seen to be identical to the one we have evaluated in Eq. (3.34), while the first integral, with the aid of Eqs. (2.11), (3.27), and (3.31), is found to be

$$\int_0^\infty dr\, r^{\lambda}\big[Q^{(0)}(r)S^{(0)}_{n_r\kappa_\lambda}(r)+P^{(0)}(r)T^{(0)}_{n_r\kappa_\lambda}(r)\big]$$
$$= -\alpha Z\left(\frac{a_0}{2Z}\right)^{\lambda+1}\frac{\sqrt{2}\,(N_{n_r\kappa_\lambda}-\kappa_\lambda)}{\sqrt{a_0|n_r|!N_{n_r\kappa_\lambda}(N_{n_r\kappa_\lambda}-\kappa_\lambda)\Gamma(2\gamma_1+1)\Gamma(|n_r|+2\gamma_{\kappa_\lambda}+1)}}\frac{\Gamma(\gamma_{\kappa_\lambda}+\gamma_1+\lambda+1)\Gamma(|n_r|+\gamma_{\kappa_\lambda}-\gamma_1-\lambda)}{\Gamma(\gamma_{\kappa_\lambda}-\gamma_1-\lambda)}. \tag{4.39}$$

Plugging Eqs. (4.39) and (3.34) into Eq. (4.38), then transforming the resulting series $\sum_{n_r=-\infty}^{\infty}(\cdots)$ into a one of the sort $\sum_{n_r=0}^{\infty}(\cdots)$, and identifying subsequently the two ${}_3F_2(1)$ functions, yields the cross susceptibility $\alpha_{\mathrm{EL}\to\mathrm{M}\lambda}$ in the form

$$\alpha_{\mathrm{EL}\to\mathrm{M}\lambda} = \frac{\alpha a_0^{\lambda+L+1}}{Z^{\lambda+L+1}}\frac{\lambda(\lambda-L)\Gamma(\gamma_{\kappa_\lambda}+\gamma_1+\lambda+1)\Gamma(\gamma_{\kappa_\lambda}+\gamma_1+L+1)}{2^{\lambda+L}(2\lambda+1)(2L+1)\Gamma(2\gamma_1+1)\Gamma(2\gamma_{\kappa_\lambda}+1)}$$
$$\times\left\{\frac{\gamma_1(\lambda+1)}{\gamma_{\kappa_\lambda}-\gamma_1+1}\,{}_3F_2\left(\begin{matrix}\gamma_{\kappa_\lambda}-\gamma_1-\lambda,\ \gamma_{\kappa_\lambda}-\gamma_1-L,\ \gamma_{\kappa_\lambda}-\gamma_1+1\\ \gamma_{\kappa_\lambda}-\gamma_1+2,\ 2\gamma_{\kappa_\lambda}+1\end{matrix};1\right)\right.$$
$$\left.-\frac{\gamma_{\kappa_\lambda}+\gamma_1}{\kappa_\lambda+1}\,{}_3F_2\left(\begin{matrix}\gamma_{\kappa_\lambda}-\gamma_1-\lambda,\ \gamma_{\kappa_\lambda}-\gamma_1-L,\ \gamma_{\kappa_\lambda}-\gamma_1\\ \gamma_{\kappa_\lambda}-\gamma_1+1,\ 2\gamma_{\kappa_\lambda}+1\end{matrix};1\right)\right\}\quad(\lambda=L\mp1). \tag{4.40}$$

Eliminating the second ${}_3F_2(1)$ in favor of the first one with the help of Eq. (3.38), we finally arrive at the following general expression for the cross susceptibility in question:

$$\alpha_{\mathrm{EL}\to\mathrm{M}\lambda} = \frac{\alpha a_0^{\lambda+L+1}}{Z^{\lambda+L+1}}\frac{\lambda(\lambda-L)\Gamma(2\gamma_1+\lambda+L+2)}{2^{\lambda+L}(\kappa_\lambda+1)(2\lambda+1)(2L+1)\Gamma(2\gamma_1+1)}$$
$$\times\left\{-1+\frac{(\lambda+1)[\gamma_1(\kappa_\lambda+1)+L+1]\Gamma(\gamma_{\kappa_\lambda}+\gamma_1+\lambda+1)\Gamma(\gamma_{\kappa_\lambda}+\gamma_1+L+1)}{(\gamma_{\kappa_\lambda}-\gamma_1+1)\Gamma(2\gamma_1+\lambda+L+2)\Gamma(2\gamma_{\kappa_\lambda}+1)}\right.$$
$$\left.\times\,{}_3F_2\left(\begin{matrix}\gamma_{\kappa_\lambda}-\gamma_1-\lambda,\ \gamma_{\kappa_\lambda}-\gamma_1-L,\ \gamma_{\kappa_\lambda}-\gamma_1+1\\ \gamma_{\kappa_\lambda}-\gamma_1+2,\ 2\gamma_{\kappa_\lambda}+1\end{matrix};1\right)\right\}\quad(\lambda=L\mp1), \tag{4.41}$$

where, we recall, κ_λ has been defined in Eq. (4.34). If in the above formula the explicit values of λ and κ_λ are set, this gives explicitly

$$\alpha_{\mathrm{EL}\to\mathrm{M}(L-1)} = \frac{\alpha a_0^{2L}}{Z^{2L}}\frac{(L-1)\Gamma(2\gamma_1+2L+1)}{2^{2L-1}(L+1)(4L^2-1)\Gamma(2\gamma_1+1)}\left\{1-\frac{L(L+1)(\gamma_1+1)\Gamma(\gamma_L+\gamma_1+L)\Gamma(\gamma_L+\gamma_1+L+1)}{(\gamma_L-\gamma_1+1)\Gamma(2\gamma_1+2L+1)\Gamma(2\gamma_L+1)}\right.$$
$$\left.\times\,{}_3F_2\left(\begin{matrix}\gamma_L-\gamma_1-L,\ \gamma_L-\gamma_1-L+1,\ \gamma_L-\gamma_1+1\\ \gamma_L-\gamma_1+2,\ 2\gamma_L+1\end{matrix};1\right)\right\} \tag{4.42}$$

and

$$\alpha_{\mathrm{EL}\to\mathrm{M}(L+1)} = \frac{\alpha a_0^{2L+2}}{Z^{2L+2}}\frac{(L+1)\Gamma(2\gamma_1+2L+3)}{2^{2L+1}L(2L+1)(2L+3)\Gamma(2\gamma_1+1)}$$
$$\times\left\{1+\frac{(L+2)(L\gamma_1-L-1)\Gamma(\gamma_{L+1}+\gamma_1+L+1)\Gamma(\gamma_{L+1}+\gamma_1+L+2)}{(\gamma_{L+1}-\gamma_1+1)\Gamma(2\gamma_1+2L+3)\Gamma(2\gamma_{L+1}+1)}\right.$$
$$\left.\times\,{}_3F_2\left(\begin{matrix}\gamma_{L+1}-\gamma_1-L-1,\ \gamma_{L+1}-\gamma_1-L,\ \gamma_{L+1}-\gamma_1+1\\ \gamma_{L+1}-\gamma_1+2,\ 2\gamma_{L+1}+1\end{matrix};1\right)\right\}. \tag{4.43}$$

TABLE IV. The static electric-to-magnetic multipole cross susceptibilities $\alpha_{\mathrm{E}L\to\mathrm{M}(L-1)}$ with $2 \leqslant L \leqslant 4$ for selected hydrogenic ions in the ground state, computed from the analytical formula in Eq. (4.42). 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	$\alpha_{\mathrm{E2}\to\mathrm{M1}}$ (units of a_0^4)	$\alpha_{\mathrm{E3}\to\mathrm{M2}}$ (units of a_0^6)	$\alpha_{\mathrm{E4}\to\mathrm{M3}}$ (units of a_0^8)
1	7.447 801 428 7 (51) $\times 10^{-8}$	7.840 878 107 8 (53) $\times 10^{-7}$	1.234 923 524 98 (84) $\times 10^{-5}$
2	1.861 763 994 3 (13) $\times 10^{-8}$	4.899 814 158 6 (34) $\times 10^{-8}$	1.929 209 479 8 (13) $\times 10^{-7}$
5	2.976 734 913 0 (21) $\times 10^{-9}$	1.253 036 091 45 (85) $\times 10^{-9}$	7.891 765 327 7 (54) $\times 10^{-10}$
10	7.423 191 448 8 (51) $\times 10^{-10}$	7.802 108 784 5 (53) $\times 10^{-11}$	1.227 360 291 30 (83) $\times 10^{-11}$
20	1.837 121 846 2 (13) $\times 10^{-10}$	4.803 053 653 1 (32) $\times 10^{-12}$	1.882 114 263 5 (13) $\times 10^{-13}$
40	4.404 779 739 7 (29) $\times 10^{-11}$	2.820 265 342 7 (18) $\times 10^{-13}$	2.722 166 133 1 (17) $\times 10^{-15}$
60	1.816 173 088 1 (11) $\times 10^{-11}$	4.983 382 447 9 (29) $\times 10^{-14}$	2.082 589 394 7 (12) $\times 10^{-16}$
80	9.069 233 476 7 (50) $\times 10^{-12}$	1.323 207 519 24 (64) $\times 10^{-14}$	2.987 634 353 8 (14) $\times 10^{-17}$
100	4.810 527 179 2 (20) $\times 10^{-12}$	4.126 084 143 0 (12) $\times 10^{-15}$	5.611 810 738 7 (12) $\times 10^{-18}$
120	2.398 905 441 474 (94) $\times 10^{-12}$	1.243 760 509 44 (27) $\times 10^{-15}$	1.064 754 960 93 (42) $\times 10^{-18}$
137	6.535 200 35 (19) $\times 10^{-13}$	1.835 801 306 (67) $\times 10^{-16}$	9.459 904 27 (40) $\times 10^{-20}$

In the particular case of the dipole ($L = 1$) perturbing electric field, the right-hand side of Eq. (4.42) vanishes, while Eq. (4.43) becomes

$$\alpha_{\mathrm{E1}\to\mathrm{M2}} = \frac{\alpha a_0^4}{Z^4}\frac{\Gamma(2\gamma_1+5)}{60\Gamma(2\gamma_1+1)}\left\{1 + \frac{3(\gamma_1-2)\Gamma(\gamma_2+\gamma_1+2)\Gamma(\gamma_2+\gamma_1+3)}{(\gamma_2-\gamma_1+1)\Gamma(2\gamma_1+5)\Gamma(2\gamma_2+1)}\,{}_3F_2\left(\begin{matrix}\gamma_2-\gamma_1-2,\ \gamma_2-\gamma_1-1,\ \gamma_2-\gamma_1+1\\ \gamma_2-\gamma_1+2,\ 2\gamma_2+1\end{matrix};1\right)\right\}. \tag{4.44}$$

With the use of the relation (3.38), the latter formula may be transformed into

$$\alpha_{\mathrm{E1}\to\mathrm{M2}} = \frac{\alpha a_0^4}{Z^4}\frac{\Gamma(2\gamma_1+5)}{240\Gamma(2\gamma_1)}\left\{1 - \frac{(\gamma_1-2)(\gamma_2+\gamma_1)\Gamma(\gamma_2+\gamma_1+2)\Gamma(\gamma_2+\gamma_1+3)}{\gamma_1\Gamma(2\gamma_1+5)\Gamma(2\gamma_2+1)}\,{}_3F_2\left(\begin{matrix}\gamma_2-\gamma_1-2,\ \gamma_2-\gamma_1-1,\ \gamma_2-\gamma_1\\ \gamma_2-\gamma_1+1,\ 2\gamma_2+1\end{matrix};1\right)\right\}, \tag{4.45}$$

which is identical to the one we have arrived at in Ref. [23, Eq. (4.24)].

Numerical values of the cross susceptibilities $\alpha_{\mathrm{E}L\to\mathrm{M}(L\mp1)}$ with $1 \leqslant L \leqslant 4$ for selected hydrogenic ions, computed from Eqs. (4.42) and (4.43), are presented in Tables IV and V.

A derivation of quasirelativistic approximations to the two cross susceptibilities $\alpha_{\mathrm{E}L\to\mathrm{M}(L\mp1)}$ is very much analogous to the procedure we have adopted in Sec. III for the polarizabilities α_L. Exploiting the relations (3.43) and (3.44), one deduces the estimates

$${}_3F_2\left(\begin{matrix}\gamma_L-\gamma_1-L,\ \gamma_L-\gamma_1-L+1,\ \gamma_L-\gamma_1+1\\ \gamma_L-\gamma_1+2,\ 2\gamma_L+1\end{matrix};1\right) \simeq 1-(\alpha Z)^2\frac{L-1}{2(L+1)(2L+1)} \tag{4.46}$$

TABLE V. The static electric-to-magnetic multipole cross susceptibilities $\alpha_{\mathrm{E}L\to\mathrm{M}(L+1)}$ with $1 \leqslant L \leqslant 4$ for selected hydrogenic ions in the ground state, computed from the analytical formula in Eq. (4.43). 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	$\alpha_{\mathrm{E1}\to\mathrm{M2}}$ (units of a_0^4)	$\alpha_{\mathrm{E2}\to\mathrm{M3}}$ (units of a_0^6)	$\alpha_{\mathrm{E3}\to\mathrm{M4}}$ (units of a_0^8)	$\alpha_{\mathrm{E4}\to\mathrm{M5}}$ (units of a_0^{10})
1	3.283 609 988 21 (74) $\times 10^{-2}$	1.641 779 910 28 (37) $\times 10^{-1}$	1.915 387 218 71 (44)	3.878 621 704 27 (88) $\times 10^{1}$
2	2.051 883 757 57 (47) $\times 10^{-3}$	2.564 697 947 34 (58) $\times 10^{-3}$	7.480 014 760 8 (17) $\times 10^{-3}$	3.786 611 359 32 (86) $\times 10^{-2}$
5	5.246 149 090 0 (12) $\times 10^{-5}$	1.048 828 974 42 (24) $\times 10^{-5}$	4.893 086 196 1 (11) $\times 10^{-6}$	3.962 443 793 36 (90) $\times 10^{-6}$
10	3.263 961 669 54 (73) $\times 10^{-6}$	1.629 485 276 85 (36) $\times 10^{-7}$	1.898 813 208 63 (42) $\times 10^{-8}$	3.841 383 757 26 (86) $\times 10^{-9}$
20	2.002 912 101 25 (43) $\times 10^{-7}$	2.488 285 199 83 (53) $\times 10^{-9}$	7.222 989 034 9 (15) $\times 10^{-11}$	3.642 467 546 25 (76) $\times 10^{-12}$
40	1.160 561 045 67 (21) $\times 10^{-8}$	3.536 787 823 83 (59) $\times 10^{-11}$	2.529 227 814 95 (40) $\times 10^{-13}$	3.150 752 599 06 (48) $\times 10^{-15}$
60	2.001 899 182 26 (22) $\times 10^{-9}$	2.622 086 172 86 (22) $\times 10^{-12}$	8.120 641 172 46 (49) $\times 10^{-15}$	4.402 352 754 59 (19) $\times 10^{-17}$
80	5.112 923 654 384 (67) $\times 10^{-10}$	3.576 878 765 05 (25) $\times 10^{-13}$	5.987 127 613 93 (69) $\times 10^{-16}$	1.767 496 114 01 (27) $\times 10^{-18}$
100	1.497 342 934 87 (38) $\times 10^{-10}$	6.199 237 022 9 (23) $\times 10^{-14}$	6.253 163 632 3 (28) $\times 10^{-17}$	1.125 356 310 60 (58) $\times 10^{-19}$
120	4.025 596 828 3 (36) $\times 10^{-11}$	1.018 161 258 7 (12) $\times 10^{-14}$	6.466 767 859 0 (85) $\times 10^{-18}$	7.469 936 050 (11) $\times 10^{-21}$
137	4.095 281 71 (19) $\times 10^{-12}$	5.745 732 04 (32) $\times 10^{-16}$	2.193 610 03 (14) $\times 10^{-19}$	1.601 547 89 (11) $\times 10^{-22}$

and

$$ {}_3F_2\left(\begin{matrix}\gamma_{L+1}-\gamma_1-L-1,\,\gamma_{L+1}-\gamma_1-L,\,\gamma_{L+1}-\gamma_1+1\\ \gamma_{L+1}-\gamma_1+2,\,2\gamma_{L+1}+1\end{matrix};1\right)\simeq 1-(\alpha Z)^2\frac{L}{2(L+2)(2L+3)}. \tag{4.47}$$

When the approximation (4.46) is inserted into Eq. (4.42), after some play with the recurrence relation (3.50), one finds that

$$\alpha_{\mathrm{E}L\to\mathrm{M}(L-1)}\simeq\frac{\alpha a_0^{2L}}{Z^{2L}}(\alpha Z)^2\frac{(L-1)^2(2L^3+5L^2+4L+2)(2L-2)!}{2^{2L}L(L+1)(2L+1)}. \tag{4.48}$$

Similarly, combining Eqs. (4.43) and (4.47) yields

$$\alpha_{\mathrm{E}L\to\mathrm{M}(L+1)}\simeq\frac{\alpha a_0^{2L+2}}{Z^{2L+2}}\frac{(L+2)(2L+2)!}{2^{2L+2}L}\left\{1-(\alpha Z)^2\left[\psi(2L+4)-\psi(2)-\frac{L(2L^4+9L^3+17L^2+17L+8)}{2(L+1)^2(L+2)(2L+1)(2L+3)}\right]\right\}. \tag{4.49}$$

It is worthwhile to notice that irrespective of the value assumed by L, the cross susceptibility $\alpha_{\mathrm{E}L\to\mathrm{M}(L-1)}$ (hence, also the induced moment $\mathsf{M}^{(1)}_{L-1}$) vanishes as $\alpha Z\to 0$, while in the same limit both $\alpha_{\mathrm{E}L\to\mathrm{M}(L+1)}$ and $\mathsf{M}^{(1)}_{L+1}$ remain finite.

Explicit forms of the expressions standing on the right-hand sides of Eqs. (4.48) and (4.49), with L restricted to the range $1\leqslant L\leqslant 4$, are collected in Table VI.

V. MAGNETIC TOROIDAL MULTIPOLE MOMENTS OF THE ATOM IN THE MULTIPOLE ELECTRIC FIELD AND ATOMIC EL → TL MULTIPOLE CROSS SUSCEPTIBILITIES

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

The last member of the family of far-field atomic multipole moments we wish to consider in this work are the magnetic toroidal moments. We show in Appendix C that spherical components of the 2^{λ}-pole magnetic toroidal moment T_{λ} due to a solenoidal current density $\boldsymbol{j}(\boldsymbol{r})$ may be written in several equivalent forms, out of which, for the use in this section, we choose the following one:

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

Proceeding along the route sketched in Sec. IV, after the current is approximated as in Eq. (4.6), we obtain

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

where

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

TABLE VI. Quasirelativistic approximations for the static electric-to-magnetic multipole cross susceptibilities $\alpha_{\mathrm{E}L\to\mathrm{M}(L-1)}$ with $2\leqslant L\leqslant 4$ and $\alpha_{\mathrm{E}L\to\mathrm{M}(L+1)}$ with $1\leqslant L\leqslant 4$ for the Dirac one-electron atom in the ground state. The expressions have been derived from Eqs. (4.48) and (4.49).

L	$\alpha_{\mathrm{E}L\to\mathrm{M}(L-1)}$	$\alpha_{\mathrm{E}L\to\mathrm{M}(L+1)}$
1		$\frac{\alpha a_0^4}{Z^4}\frac{9}{2}\left[1-\frac{409}{360}(\alpha Z)^2\right]$
2	$\frac{\alpha a_0^4}{Z^4}\frac{23}{120}(\alpha Z)^2$	$\frac{\alpha a_0^6}{Z^6}\frac{45}{2}\left[1-\frac{1793}{1260}(\alpha Z)^2\right]$
3	$\frac{\alpha a_0^6}{Z^6}\frac{113}{56}(\alpha Z)^2$	$\frac{\alpha a_0^8}{Z^8}\frac{525}{2}\left[1-\frac{3317}{2016}(\alpha Z)^2\right]$
4	$\frac{\alpha a_0^8}{Z^8}\frac{1017}{32}(\alpha Z)^2$	$\frac{\alpha a_0^{10}}{Z^{10}}\frac{42525}{8}\left[1-\frac{759449}{415800}(\alpha Z)^2\right]$

and

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

with $\boldsymbol{j}^{(0)}(\boldsymbol{r})$ and $\boldsymbol{j}^{(1)}(\boldsymbol{r})$ given, respectively, by Eqs. (4.7) and (4.8).

At first, we show that in the ground state of an isolated atom all permanent toroidal multipole moments do vanish. To this end, we insert the expression (4.7) for $\boldsymbol{j}^{(0)}(\boldsymbol{r})$ into the right-hand side of Eq. (5.3) and then make use of Eqs. (2.9) and (2.10), together with the identity [36, Eq. (3.1.3)]

$$\boldsymbol{n}_r\cdot\boldsymbol{\sigma}\,\Omega_{\kappa m_\kappa}(\boldsymbol{n}_r)=-\Omega_{-\kappa m_\kappa}(\boldsymbol{n}_r), \tag{5.5}$$

obtaining

$$\begin{aligned}\mathcal{T}^{(0)}_{\lambda\mu}&=\frac{iec}{\lambda+1}\sqrt{\frac{4\pi}{2\lambda+1}}\int_0^{\infty}dr\,r^{\lambda+1}P^{(0)}(r)Q^{(0)}(r)\\&\quad\times\sum_{m=-1/2}^{1/2}\sum_{m'=-1/2}^{1/2}a_m^*a_{m'}[\langle\Omega_{-1m}|Y_{\lambda\mu}\Omega_{-1m'}\rangle\\&\quad-\langle\Omega_{1m}|Y_{\lambda\mu}\Omega_{1m'}\rangle].\end{aligned} \tag{5.6}$$

It follows from the property displayed in Eq. (2.20) [being, in fact, the consequence of the identity (5.5)] that for all λ, μ, m, and m' the expression in the square bracket on the right-hand side of the above equation is zero. Hence, we arrive at the aforementioned result

$$\mathcal{T}^{(0)}_{\lambda\mu}=0. \tag{5.7}$$

Next, we turn our attention to the first-order induced moments $\mathsf{T}^{(1)}_{\lambda}$. From Eqs. (5.4), (4.8), and (3.10), we have

$$\mathcal{T}^{(1)}_{\lambda\mu}=\widetilde{\mathcal{T}}^{(1)}_{\lambda\mu}+(-)^{\mu}\widetilde{\mathcal{T}}^{(1)*}_{\lambda,-\mu}, \tag{5.8}$$

with

$$\begin{aligned}\widetilde{\mathcal{T}}^{(1)}_{\lambda\mu}&=-\frac{ec}{\lambda+1}\sqrt{\frac{4\pi}{2\lambda+1}}\\&\quad\times\int_{\mathbb{R}^3}d^3\boldsymbol{r}\,r^{\lambda+1}Y_{\lambda\mu}(\boldsymbol{n}_r)\Psi^{(0)\dagger}(\boldsymbol{r})\boldsymbol{n}_r\cdot\boldsymbol{\alpha}\Psi^{(1)}(\boldsymbol{r}).\end{aligned} \tag{5.9}$$

Skipping details that should be already obvious to the reader who has gone through Secs. III and IV, we come to the inference that Eq. (5.9) may be converted into

$$\widetilde{\mathcal{T}}_{\lambda\mu}^{(1)} = \frac{i(4\pi\epsilon_0)c}{\lambda+1}\frac{4\pi}{\sqrt{(2\lambda+1)(2L+1)}}\sum_{\substack{\kappa=-\infty \\ (\kappa\neq 0)}}^{\infty} R_{\kappa}^{(\lambda+1,L)}(Q^{(0)},-P^{(0)};P^{(0)},Q^{(0)})$$
$$\times\sum_{M=-L}^{L}\sum_{m_\kappa=-|\kappa|+1/2}^{|\kappa|-1/2}\sum_{m=-1/2}^{1/2}\sum_{m'=-1/2}^{1/2} a_m^* a_{m'} \mathcal{C}_{LM}^{(1)*}\langle\Omega_{-1m}|Y_{\lambda\mu}\Omega_{\kappa m_\kappa}\rangle\langle\Omega_{\kappa m_\kappa}|Y_{LM}\Omega_{-1m'}\rangle. \tag{5.10}$$

Comparison of the multiple sum on the right-hand side of Eq. (5.10) with the one that appears in Eq. (3.14) shows that the two are identical. This allows us to save labor, and, after exploiting results of Sec. III A, we quickly find that

$$\mathcal{T}_{\lambda\mu}^{(1)} = \mathcal{T}_{\lambda\mu}^{(1)}\delta_{\lambda L}, \tag{5.11}$$

where

$$\mathcal{T}_{L\mu}^{(1)} = \mathcal{T}_{L\mu,L}^{(1)} + \mathcal{T}_{L\mu,-L-1}^{(1)}, \tag{5.12}$$

with

$$\mathcal{T}_{L\mu,\kappa}^{(1)} = (4\pi\epsilon_0)c\frac{2i\,\mathrm{sgn}(\kappa)}{(L+1)(2L+1)^2}R_{\kappa}^{(L+1,L)}(Q^{(0)},-P^{(0)};P^{(0)},Q^{(0)})$$
$$\times\left[\mu(|a_{1/2}|^2-|a_{-1/2}|^2)\mathcal{C}_{L\mu}^{(1)}+\sqrt{(L-\mu)(L+\mu+1)}\,a_{1/2}a_{-1/2}^*\mathcal{C}_{L,\mu+1}^{(1)}+\sqrt{(L+\mu)(L-\mu+1)}\,a_{1/2}^*a_{-1/2}\mathcal{C}_{L,\mu-1}^{(1)}\right]$$
$$(\kappa = L,-L-1). \tag{5.13}$$

In Sec. IV A, we have succeeded in expressing the two induced magnetic moments $\mathsf{M}_{L\mp1}^{(1)}$ in terms of certain irreducible tensor products of the vector (rank 1 tensor) $\boldsymbol{\nu}$, introduced in Eq. (4.15), and the 2^L-pole tensor $\mathsf{C}_L^{(1)}$, characterizing the perturbing electrostatic field. An analogous simplification is possible in the case of the toroidal moments considered here. Invoking Eq. (4.15) and rewriting the right-hand side of Eq. (5.13) in terms of the spherical components of the vector $\boldsymbol{\nu}$, after making use of a table of the Clebsch-Gordan coefficients [40, Table 8.2], we arrive at

$$\mathcal{T}_{L\mu,\kappa}^{(1)} = -(4\pi\epsilon_0)c\frac{2i\,\mathrm{sgn}(\kappa)}{(2L+1)^2}\sqrt{\frac{L}{L+1}}R_{\kappa}^{(L+1,L)}(Q^{(0)},-P^{(0)};P^{(0)},Q^{(0)})\{\boldsymbol{\nu}\otimes\mathsf{C}_L^{(1)}\}_{L\mu} \quad (\kappa = L,-L-1). \tag{5.14}$$

In summary, in this section we have shown that in the ground state of an isolated atom all magnetic toroidal multipole moments due to the electronic movement vanish, while, to the first order of approximation, a perturbing 2^L-pole static electric field induces the toroidal moment of the same multipolar symmetry as that of the perturbing field, i.e.,

$$\mathsf{T}_\lambda \simeq \mathsf{T}_\lambda^{(1)}\delta_{\lambda L}. \tag{5.15}$$

B. Atomic multipole EL → TL cross susceptibilities

We define the atomic multipole electric-to-magnetic toroidal cross susceptibilities $\alpha_{\mathrm{E}L\to\mathrm{T}L}$ according to

$$\mathsf{T}_L^{(1)} = i(4\pi\epsilon_0)c\,\alpha_{\mathrm{E}L\to\mathrm{T}L}\sqrt{L(L+1)}\,\{\boldsymbol{\nu}\otimes\mathsf{C}_L^{(1)}\}_L. \tag{5.16}$$

Comparison of Eq. (5.16) with Eqs. (5.12) and (5.14) gives $\alpha_{\mathrm{E}L\to\mathrm{T}L}$ in the form of the sum

$$\alpha_{\mathrm{E}L\to\mathrm{T}L} = \alpha_{\mathrm{E}L\to\mathrm{T}L,L} + \alpha_{\mathrm{E}L\to\mathrm{T}L,-L-1}, \tag{5.17}$$

with the two addends given by

$$\alpha_{\mathrm{E}L\to\mathrm{T}L,\kappa} = -\frac{2\,\mathrm{sgn}(\kappa)}{(L+1)(2L+1)^2}R_{\kappa}^{(L+1,L)}(Q^{(0)},-P^{(0)};P^{(0)},Q^{(0)}) \quad (\kappa = L,-L-1) \tag{5.18}$$

or, by virtue of the definition (3.15) and the expansion (3.26), by

$$\alpha_{\mathrm{E}L\to\mathrm{T}L,\kappa} = -\frac{2\,\mathrm{sgn}(\kappa)}{(L+1)(2L+1)^2}\sum_{n_r=-\infty}^{\infty}\frac{1}{\mu_{n_r\kappa}^{(0)}-1}\int_0^\infty dr\,r^{L+1}\left[Q^{(0)}(r)S_{n_r\kappa}^{(0)}(r)-P^{(0)}(r)T_{n_r\kappa}^{(0)}(r)\right]$$
$$\times\int_0^\infty dr'\,r'^L\left[\mu_{n_r\kappa}^{(0)}P^{(0)}(r')S_{n_r\kappa}^{(0)}(r')+Q^{(0)}(r')T_{n_r\kappa}^{(0)}(r')\right] \quad (\kappa = L,-L-1). \tag{5.19}$$

The integral over r' is seen to be identical to the one evaluated in Eq. (3.34), while the one over r, after the use is made of Eqs. (3.27) and (3.31), is found to be

$$\int_0^\infty dr r^{L+1}\left[Q^{(0)}(r)S^{(0)}_{n_r\kappa}(r) - P^{(0)}(r)T^{(0)}_{n_r\kappa}(r)\right]$$
$$= \alpha Z\left(\frac{a_0}{2Z}\right)^{L+2}\frac{\sqrt{2}\,|n_r|(|n_r|+2\gamma_\kappa)}{\sqrt{a_0|n_r|!N_{n_r\kappa}(N_{n_r\kappa}-\kappa)\Gamma(2\gamma_1+1)\Gamma(|n_r|+2\gamma_\kappa+1)}}\frac{\Gamma(\gamma_\kappa+\gamma_1+L+2)\Gamma(|n_r|+\gamma_\kappa-\gamma_1-L-2)}{\Gamma(\gamma_\kappa-\gamma_1-L-1)}. \tag{5.20}$$

Inserting Eqs. (3.34) and (5.20) into the right-hand side of Eq. (5.19) and summing the resulting series, with the same procedure we have applied before in Secs. III B and IV B, to a form involving a particular ${}_3F_2(1)$ function, yields the following general expression for $\alpha_{\mathrm{E}L\to\mathrm{T}L,\kappa}$:

$$\alpha_{\mathrm{E}L\to\mathrm{T}L,\kappa} = \frac{\alpha a_0^{2L+2}}{Z^{2L+2}}\frac{\mathrm{sgn}(\kappa)[\gamma_1(\kappa+1)+L+1]\Gamma(\gamma_\kappa+\gamma_1+L+1)\Gamma(\gamma_\kappa+\gamma_1+L+2)}{2^{2L+1}(L+1)(2L+1)^2(\gamma_\kappa-\gamma_1+1)\Gamma(2\gamma_1+1)\Gamma(2\gamma_\kappa+1)}$$
$$\times\,{}_3F_2\left(\begin{matrix}\gamma_\kappa-\gamma_1-L-1,\,\gamma_\kappa-\gamma_1-L,\,\gamma_\kappa-\gamma_1+1\\ \gamma_\kappa-\gamma_1+2,\,2\gamma_\kappa+1\end{matrix};1\right)\quad(\kappa=L,-L-1). \tag{5.21}$$

Hence, we find that the cross susceptibility $\alpha_{\mathrm{E}L\to\mathrm{T}L}$ is the sum of

$$\alpha_{\mathrm{E}L\to\mathrm{T}L,L} = \frac{\alpha a_0^{2L+2}}{Z^{2L+2}}\frac{(\gamma_1+1)\Gamma(\gamma_L+\gamma_1+L+1)\Gamma(\gamma_L+\gamma_1+L+2)}{2^{2L+1}(2L+1)^2(\gamma_L-\gamma_1+1)\Gamma(2\gamma_1+1)\Gamma(2\gamma_L+1)}$$
$$\times\,{}_3F_2\left(\begin{matrix}\gamma_L-\gamma_1-L-1,\,\gamma_L-\gamma_1-L,\,\gamma_L-\gamma_1+1\\ \gamma_L-\gamma_1+2,\,2\gamma_L+1\end{matrix};1\right) \tag{5.22a}$$

and

$$\alpha_{\mathrm{E}L\to\mathrm{T}L,-L-1} = \frac{\alpha a_0^{2L+2}}{Z^{2L+2}}\frac{(L\gamma_1-L-1)\Gamma(\gamma_{L+1}+\gamma_1+L+1)\Gamma(\gamma_{L+1}+\gamma_1+L+2)}{2^{2L+1}(L+1)(2L+1)^2(\gamma_{L+1}-\gamma_1+1)\Gamma(2\gamma_1+1)\Gamma(2\gamma_{L+1}+1)}$$
$$\times\,{}_3F_2\left(\begin{matrix}\gamma_{L+1}-\gamma_1-L-1,\,\gamma_{L+1}-\gamma_1-L,\,\gamma_{L+1}-\gamma_1+1\\ \gamma_{L+1}-\gamma_1+2,\,2\gamma_{L+1}+1\end{matrix};1\right); \tag{5.22b}$$

i.e., one has

$$\alpha_{\mathrm{E}L\to\mathrm{T}L} = \frac{\alpha a_0^{2L+2}}{Z^{2L+2}}\frac{1}{2^{2L+1}(2L+1)^2\Gamma(2\gamma_1+1)}\left\{\frac{(\gamma_1+1)\Gamma(\gamma_L+\gamma_1+L+1)\Gamma(\gamma_L+\gamma_1+L+2)}{(\gamma_L-\gamma_1+1)\Gamma(2\gamma_L+1)}\right.$$
$$\times\,{}_3F_2\left(\begin{matrix}\gamma_L-\gamma_1-L-1,\,\gamma_L-\gamma_1-L,\,\gamma_L-\gamma_1+1\\ \gamma_L-\gamma_1+2,\,2\gamma_L+1\end{matrix};1\right)$$
$$+\frac{(L\gamma_1-L-1)\Gamma(\gamma_{L+1}+\gamma_1+L+1)\Gamma(\gamma_{L+1}+\gamma_1+L+2)}{(L+1)(\gamma_{L+1}-\gamma_1+1)\Gamma(2\gamma_{L+1}+1)}$$
$$\left.\times\,{}_3F_2\left(\begin{matrix}\gamma_{L+1}-\gamma_1-L-1,\,\gamma_{L+1}-\gamma_1-L,\,\gamma_{L+1}-\gamma_1+1\\ \gamma_{L+1}-\gamma_1+2,\,2\gamma_{L+1}+1\end{matrix};1\right)\right\}. \tag{5.23}$$

Tabulation of numerical values of the cross susceptibilities $\alpha_{\mathrm{E}L\to\mathrm{T}L}$ with $1 \leqslant L \leqslant 4$ for selected hydrogenic ions is done in Table VII.

In the particular case where the perturbing electric field is of dipolar ($L = 1$) character, the first ${}_3F_2(1)$ series on the right-hand side of Eq. (5.23) is a terminating one and $\alpha_{\mathrm{E}1\to\mathrm{T}1}$ appears to have the relatively simple form

$$\alpha_{\mathrm{E}1\to\mathrm{T}1} = \frac{\alpha a_0^4}{Z^4}\left\{\frac{(\gamma_1+1)^3(2\gamma_1+1)}{18}+\frac{(\gamma_1-2)\Gamma(\gamma_2+\gamma_1+2)\Gamma(\gamma_2+\gamma_1+3)}{144(\gamma_2-\gamma_1+1)\Gamma(2\gamma_1+1)\Gamma(2\gamma_2+1)}\right.$$
$$\left.\times\,{}_3F_2\left(\begin{matrix}\gamma_2-\gamma_1-2,\,\gamma_2-\gamma_1-1,\,\gamma_2-\gamma_1+1\\ \gamma_2-\gamma_1+2,\,2\gamma_2+1\end{matrix};1\right)\right\}. \tag{5.24}$$

TABLE VII. The static electric-to-toroidal-magnetic multipole cross susceptibilities $\alpha_{EL\to TL}$ with $1 \leqslant L \leqslant 4$ for selected hydrogenic ions in the ground state, computed from the analytical formula in Eq. (5.23). 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	$\alpha_{E1\to T1}$ (units of a_0^4)	$\alpha_{E2\to T2}$ (units of a_0^6)	$\alpha_{E3\to T3}$ (units of a_0^8)	$\alpha_{E4\to T4}$ (units of a_0^{10})
1	8.208 992 048 8 (19) $\times 10^{-3}$	1.824 181 749 47 (41) $\times 10^{-2}$	1.197 103 615 58 (28) $\times 10^{-1}$	1.551 430 471 54 (35)
2	5.129 627 095 4 (12) $\times 10^{-4}$	2.849 550 959 88 (65) $\times 10^{-4}$	4.674 799 949 9 (11) $\times 10^{-4}$	1.514 573 425 52 (34) $\times 10^{-3}$
5	1.311 405 660 90 (30) $\times 10^{-5}$	1.165 075 455 46 (27) $\times 10^{-6}$	3.057 322 790 70 (69) $\times 10^{-7}$	1.584 512 136 37 (36) $\times 10^{-7}$
10	8.156 619 781 8 (19) $\times 10^{-7}$	1.808 732 920 30 (41) $\times 10^{-8}$	1.185 426 820 77 (27) $\times 10^{-9}$	1.534 745 348 09 (34) $\times 10^{-10}$
20	4.999 128 489 4 (11) $\times 10^{-8}$	2.753 638 596 01 (58) $\times 10^{-10}$	4.493 949 807 48 (94) $\times 10^{-12}$	1.450 075 102 23 (30) $\times 10^{-13}$
40	2.881 625 203 51 (51) $\times 10^{-9}$	3.864 378 956 52 (62) $\times 10^{-12}$	1.551 228 291 91 (23) $\times 10^{-14}$	1.235 602 013 60 (18) $\times 10^{-16}$
60	4.921 478 469 93 (50) $\times 10^{-10}$	2.797 665 976 33 (17) $\times 10^{-13}$	4.849 315 540 87 (18) $\times 10^{-16}$	1.678 687 380 721 (30) $\times 10^{-18}$
80	1.235 279 761 024 (42) $\times 10^{-10}$	3.666 029 498 03 (43) $\times 10^{-14}$	3.417 412 738 36 (57) $\times 10^{-17}$	6.427 122 689 3 (13) $\times 10^{-20}$
100	3.504 059 007 8 (11) $\times 10^{-11}$	5.922 743 695 6 (28) $\times 10^{-15}$	3.298 079 781 3 (19) $\times 10^{-18}$	3.764 776 924 1 (24) $\times 10^{-21}$
120	8.770 433 963 4 (93) $\times 10^{-12}$	8.385 272 052 (12) $\times 10^{-16}$	2.882 550 881 2 (48) $\times 10^{-19}$	2.089 625 125 2 (39) $\times 10^{-22}$
137	5.927 356 55 (38) $\times 10^{-13}$	2.011 157 10 (19) $\times 10^{-17}$	3.384 692 32 (40) $\times 10^{-21}$	1.335 922 79 (18) $\times 10^{-24}$

The dipolar case was studied by our group a decade ago in Ref. [25], where the following representation of $\alpha_{E1\to T1}$ was derived[5]:

$$\alpha_{E1\to T1} = \frac{\alpha a_0^4}{Z^4}\left\{\frac{(\gamma_1+1)(2\gamma_1+1)\left(8\gamma_1^3+54\gamma_1^2+67\gamma_1+18\right)}{864} - \frac{(\gamma_1-2)(4\gamma_1+1)\Gamma^2(\gamma_2+\gamma_1+2)}{576(\gamma_2-\gamma_1)\Gamma(2\gamma_1+1)\Gamma(2\gamma_2+1)} \times {}_3F_2\left(\begin{matrix}\gamma_2-\gamma_1-1,\,\gamma_2-\gamma_1-1,\,\gamma_2-\gamma_1\\ \gamma_2-\gamma_1+1,\,2\gamma_2+1\end{matrix};1\right)\right\}. \tag{5.25}$$

Equivalence of the expressions in Eqs. (5.24) and (5.25) may be proved with the aid of the identity

$$ {}_3F_2\left(\begin{matrix}a_1,\,a_2,\,a_3\\ a_3+1,\,b\end{matrix};1\right) = \left[1-\frac{(a_1-a_3-1)(a_2-a_3-1)}{(a_1-1)(b-a_1)}\right]\frac{\Gamma(b)\Gamma(b-a_1-a_2+1)}{(b-a_3-1)\Gamma(b-a_1)\Gamma(b-a_2)} - \frac{(a_1-a_3-1)(a_1-a_3-2)(a_2-a_3-1)}{(a_1-1)(a_3+1)(b-a_3-1)}\,{}_3F_2\left(\begin{matrix}a_1-1,\,a_2,\,a_3+1\\ a_3+2,\,b\end{matrix};1\right) \quad [\mathrm{Re}(b-a_1-a_2)>1]. \tag{5.26}$$

To find a quasirelativistic limit of the general expression for the cross susceptibilities under study, we approximate the hypergeometric function appearing in Eq. (5.22a) with the formula

$$ {}_3F_2\left(\begin{matrix}\gamma_L-\gamma_1-L-1,\,\gamma_L-\gamma_1-L,\,\gamma_L-\gamma_1+1\\ \gamma_L-\gamma_1+2,\,2\gamma_L+1\end{matrix};1\right) \simeq \frac{2L^2+5L+1}{(L+1)(2L+1)} - (\alpha Z)^2\frac{12L^5+32L^4-15L^3-68L^2-17L+8}{4L(L+1)^2(L+2)(2L+1)^2} \tag{5.27}$$

and the one in Eq. (5.22b) using Eq. (4.47). This yields the following estimations of the two addends in Eq. (5.17):

$$\alpha_{EL\to TL,L} \simeq \frac{\alpha a_0^{2L+2}}{Z^{2L+2}}\frac{(2L^2+5L+1)(2L)!}{2^{2L}L(2L+1)}\left\{1-(\alpha Z)^2\left[\psi(2L+2)-\psi(2)-\frac{2L^6-L^5-26L^4-31L^3+4L+4}{4L^2(L+1)(L+2)(2L^2+5L+1)}\right]\right\}, \tag{5.28a}$$

$$\alpha_{EL\to TL,-L-1} \simeq -\frac{\alpha a_0^{2L+2}}{Z^{2L+2}}\frac{(2L+3)(2L)!}{2^{2L+1}(L+1)(2L+1)}\left\{1-(\alpha Z)^2\left[\psi(2L+2)-\psi(2)-\frac{2L^5+13L^4+27L^3+18L^2-3L-4}{2(L+1)^2(L+2)(2L+3)}\right]\right\}. \tag{5.28b}$$

[5]Equation (5.25) follows from Eq. (4.32) in Ref. [25], where the expression for $\tau = c\alpha_{E1\to T1}$ was presented. The reader might be surprised that by setting $L = 1$ in Eqs. (5.22a) and (5.22b) and multiplying the results by the speed of light, one does not reproduce Eqs. (4.24) and (4.31) in Ref. [25]. The origin of this apparent paradox is that splitting the components $\mathcal{T}_{L\mu}^{(1)}$ of the induced toroidal moment into a sum of two κ-dependent addends is not (and, in fact, need not to be) unique and depends on a particular integral representation of $\mathcal{T}_{\lambda\mu}$ chosen as a starting point (in this connection, see the discussion in Appendix C). However, the sum of the two addends is, of course, always the same.

Adding the right-hand sides of Eqs. (5.28a) and (5.28b), after some algebra we arrive at the sought quasirelativistic representation of $\alpha_{\mathrm{E}L\to\mathrm{T}L}$:

$$\alpha_{\mathrm{E}L\to\mathrm{T}L} \simeq \frac{\alpha a_0^{2L+2}}{Z^{2L+2}} \frac{(L+2)(2L+1)!}{2^{2L+1}L(L+1)} \left\{ 1-(\alpha Z)^2 \left[\psi(2L+3)-\psi(2) + \frac{6L^7+29L^6+49L^5+32L^4-L^3-16L^2-12L-4}{2L^2(L+1)^2(L+2)^2(2L+1)^2} \right] \right\}. \tag{5.29}$$

Table VIII collects the quasirelativistic approximations of $\alpha_{\mathrm{E}L\to\mathrm{T}L}$ obtained from Eq. (5.29) for $1 \leqslant L \leqslant 4$.

VI. NEAR-NUCLEUS ELECTRIC MULTIPOLE MOMENTS OF THE ATOM IN THE MULTIPOLE ELECTRIC FIELD AND ELECTRIC MULTIPOLE NUCLEAR SHIELDING CONSTANTS

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

With this section, we start the second part of the paper, in which we analyze near-field (henceforth, in view of the present context, the term *near-nucleus* is used instead) multipole moments characterizing electrostatic and magnetostatic potentials and fields generated by the atomic electron in the region near a point where the atomic nucleus is located. The first of these moments is the near-nucleus electric multipole moment R_λ, the spherical components of which are defined to be

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

where $\rho(\boldsymbol{r})$ is the electronic charge density given by Eq. (3.2). Approximating the density as in Eq. (3.3) yields

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

with the permanent and the first-order induced parts given by

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

and

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

respectively.

Evaluation of both $\mathcal{R}_{\lambda\mu}^{(0)}$ and $\mathcal{R}_{\lambda\mu}^{(1)}$ is much simplified by the fact that angular integrations involved are identical to these encountered in Sec. III A, where the counterpart far-field moments $\mathcal{Q}_{\lambda\mu}^{(0)}$ and $\mathcal{Q}_{\lambda\mu}^{(1)}$ have been analyzed. In result, one finds that

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

with the nonvanishing components given by

$$\mathcal{R}_{00}^{(0)} = -e\int_0^\infty dr\, r^{-1}\{[P^{(0)}(r)]^2 + [Q^{(0)}(r)]^2\} \tag{6.6}$$

and

$$\mathcal{R}_{L\mu}^{(1)} = \mathcal{R}_{L\mu,L}^{(1)} + \mathcal{R}_{L\mu,-L-1}^{(1)}, \tag{6.7}$$

where

$$\mathcal{R}_{L\mu,\kappa}^{(1)} = (4\pi\epsilon_0)\frac{2|\kappa|}{(2L+1)^2} R_\kappa^{(-L-1,L)}(P^{(0)},Q^{(0)};P^{(0)},Q^{(0)})\mathcal{C}_{L\mu}^{(1)}$$
$$(\kappa = L, -L-1). \tag{6.8}$$

In the last equation, $R_\kappa^{(-L-1,L)}(P^{(0)},Q^{(0)};P^{(0)},Q^{(0)})$ is a particular form of the double radial integral defined in Eq. (3.15). Invoking the explicit forms (2.11) of the electronic radial functions, one immediately finds that

$$\mathcal{R}_{00}^{(0)} = -\frac{Ze}{a_0\gamma_1}. \tag{6.9}$$

B. Atomic electric multipole nuclear shielding constants

In analogy with the far-field case, the present analysis leads in a natural way to a definition of a near-nucleus electric 2^L-pole polarizability of the atom, $\sigma_{\mathrm{E}L\to\mathrm{E}L}$, through the relation

$$\mathsf{R}_L^{(1)} = (4\pi\epsilon_0)\sigma_{\mathrm{E}L\to\mathrm{E}L}\mathsf{C}_L^{(1)}. \tag{6.10}$$

In the literature, the near-nucleus polarizability $\sigma_{\mathrm{E}L\to\mathrm{E}L}$ is usually named the electric multipole nuclear shielding constant, and in what follows we adopt that nomenclature. Combining Eq. (6.10) with Eqs. (6.7) and (6.8), we deduce that

$$\sigma_{\mathrm{E}L\to\mathrm{E}L} = \sigma_{\mathrm{E}L\to\mathrm{E}L,L} + \sigma_{\mathrm{E}L\to\mathrm{E}L,-L-1}, \tag{6.11}$$

with

$$\sigma_{\mathrm{E}L\to\mathrm{E}L,\kappa} = \frac{2|\kappa|}{(2L+1)^2} R_\kappa^{(-L-1,L)}(P^{(0)},Q^{(0)};P^{(0)},Q^{(0)})$$
$$(\kappa = L, -L-1), \tag{6.12}$$

TABLE VIII. Quasirelativistic approximations for the static electric-to-toroidal-magnetic multipole cross susceptibilities $\alpha_{\mathrm{E}L\to\mathrm{T}L}$ with $1 \leqslant L \leqslant 4$ for the Dirac one-electron atom in the ground state. The expressions have been derived from Eq. (5.29).

L	$\alpha_{\mathrm{E}L\to\mathrm{T}L}$
1	$\frac{\alpha a_0^4}{Z^4}\frac{9}{8}\left[1-\frac{785}{648}(\alpha Z)^2\right]$
2	$\frac{\alpha a_0^6}{Z^6}\frac{5}{2}\left[1-\frac{11591}{7200}(\alpha Z)^2\right]$
3	$\frac{\alpha a_0^8}{Z^8}\frac{525}{32}\left[1-\frac{654611}{352800}(\alpha Z)^2\right]$
4	$\frac{\alpha a_0^{10}}{Z^{10}}\frac{1701}{8}\left[1-\frac{8356217}{4082400}(\alpha Z)^2\right]$

where, by virtue of Eqs. (3.15) and (3.26), the double radial integral may be written as

$$R_{\kappa}^{(-L-1,L)}(P^{(0)},Q^{(0)};P^{(0)},Q^{(0)}) = \sum_{n_r=-\infty}^{\infty} \frac{1}{\mu_{n_r\kappa}^{(0)}-1} \int_0^\infty dr r^{-L-1}\big[P^{(0)}(r)S_{n_r\kappa}^{(0)}(r)+Q^{(0)}(r)T_{n_r\kappa}^{(0)}(r)\big]$$
$$\times \int_0^\infty dr' r'^{L}\big[\mu_{n_r\kappa}^{(0)}P^{(0)}(r')S_{n_r\kappa}^{(0)}(r')+Q^{(0)}(r')T_{n_r\kappa}^{(0)}(r')\big] \quad (\kappa = L, -L-1). \tag{6.13}$$

As the integral over r' is the one from Eq. (3.34), while that over r is found to be

$$\int_0^\infty dr r^{-L-1}\big[P^{(0)}(r)S_{n_r\kappa}^{(0)}(r)+Q^{(0)}(r)T_{n_r\kappa}^{(0)}(r)\big]$$
$$= -\left(\frac{2Z}{a_0}\right)^L \frac{\sqrt{2}(N_{n_r\kappa}-\kappa)[\gamma_1(N_{n_r\kappa}+\kappa)-(|n_r|+\gamma_\kappa-\gamma_1+L)]}{\sqrt{a_0|n_r|!N_{n_r\kappa}(N_{n_r\kappa}-\kappa)\Gamma(2\gamma_1+1)\Gamma(|n_r|+2\gamma_\kappa+1)}} \frac{\Gamma(\gamma_\kappa+\gamma_1-L)\Gamma(|n_r|+\gamma_\kappa-\gamma_1+L)}{\Gamma(\gamma_\kappa-\gamma_1+L+1)}$$
$$\left(Z < \alpha^{-1}\frac{\sqrt{4L^2-1}}{2L} \text{ for } \kappa = L\right), \tag{6.14}$$

by means of the by now familiar procedure of summation of the series over n_r to a closed form involving a single ${}_3F_2(1)$ function, we arrive at the following expression for $\sigma_{\mathrm{EL}\to\mathrm{EL},\kappa}$:

$$\sigma_{\mathrm{EL}\to\mathrm{EL},\kappa} = \frac{2|\kappa|}{Z(\kappa+1)(2L+1)^2}\Bigg\{-1+\frac{[\gamma_1(\kappa+1)-L][\gamma_1(\kappa+1)+L+1]\Gamma(\gamma_\kappa+\gamma_1-L)\Gamma(\gamma_\kappa+\gamma_1+L+1)}{(\gamma_\kappa-\gamma_1+1)\Gamma(2\gamma_1+1)\Gamma(2\gamma_\kappa+1)}$$
$$\times {}_3F_2\left(\begin{matrix}\gamma_\kappa-\gamma_1+L+1,\ \gamma_\kappa-\gamma_1-L,\ \gamma_\kappa-\gamma_1+1\\ \gamma_\kappa-\gamma_1+2,\ 2\gamma_\kappa+1\end{matrix};1\right)\Bigg\} \quad (\kappa = L, -L-1). \tag{6.15}$$

At the first sight, the expression on the right-hand side of Eq. (6.15) looks equally complicated as its counterparts displayed in Eqs. (3.39), (4.41), and (5.21). It appears, however, that because of particular forms of the parameters in the ${}_3F_2(1)$ function being involved, it may be transformed to a much simpler representation. To this end, we exploit the identity [44, Eq. (7.4.4.1)]

$${}_3F_2\left(\begin{matrix}a_1,\ a_2,\ a_3\\ b_1,\ b_2\end{matrix};1\right) = \frac{\Gamma(b_2)\Gamma(s)}{\Gamma(b_2-a_2)\Gamma(s+a_2)}\,{}_3F_2\left(\begin{matrix}b_1-a_1,\ b_1-a_3,\ a_2\\ b_1,\ s+a_2\end{matrix};1\right)$$
$$[s = b_1+b_2-a_1-a_2-a_3;\ \mathrm{Re}\, s > 0;\ \mathrm{Re}(b_2-a_2) > 0], \tag{6.16}$$

and this casts Eq. (6.15) into

$$\sigma_{\mathrm{EL}\to\mathrm{EL},\kappa} = \frac{2|\kappa|}{Z(\kappa+1)(2L+1)^2}\left\{-1+\frac{[\gamma_1(\kappa+1)-L][\gamma_1(\kappa+1)+L+1]}{(\gamma_\kappa-\gamma_1+1)(\gamma_\kappa+\gamma_1-L)}\,{}_3F_2\left(\begin{matrix}-L+1,\ 1,\ \gamma_\kappa-\gamma_1-L\\ \gamma_\kappa-\gamma_1+2,\ \gamma_\kappa+\gamma_1-L+1\end{matrix};1\right)\right\}$$
$$(\kappa = L, -L-1). \tag{6.17}$$

Hence, the two addends on the right-hand side of Eq. (6.11) may be explicitly written as

$$\sigma_{\mathrm{EL}\to\mathrm{EL},L} = \frac{2L}{Z(L+1)(2L+1)^2}\left\{-1+\frac{(L+1)(\gamma_1+1)[\gamma_1(L+1)-L]}{(\gamma_L-\gamma_1+1)(\gamma_L+\gamma_1-L)}\,{}_3F_2\left(\begin{matrix}-L+1,\ 1,\ \gamma_L-\gamma_1-L\\ \gamma_L-\gamma_1+2,\ \gamma_L+\gamma_1-L+1\end{matrix};1\right)\right\} \tag{6.18a}$$

and

$$\sigma_{\mathrm{EL}\to\mathrm{EL},-L-1} = \frac{2(L+1)}{ZL(2L+1)^2}\left\{1-\frac{L(\gamma_1+1)(L\gamma_1-L-1)}{(\gamma_{L+1}-\gamma_1+1)(\gamma_{L+1}+\gamma_1-L)}\,{}_3F_2\left(\begin{matrix}-L+1,\ 1,\ \gamma_{L+1}-\gamma_1-L\\ \gamma_{L+1}-\gamma_1+2,\ \gamma_{L+1}+\gamma_1-L+1\end{matrix};1\right)\right\}, \tag{6.18b}$$

and consequently the sought formula for the 2^L-pole electric shielding constants is

$$\sigma_{\mathrm{EL}\to\mathrm{EL}} = \frac{2}{ZL(L+1)(2L+1)}\Bigg\{1+\frac{L^2(L+1)(\gamma_1+1)[\gamma_1(L+1)-L]}{(2L+1)(\gamma_L-\gamma_1+1)(\gamma_L+\gamma_1-L)}\,{}_3F_2\left(\begin{matrix}-L+1,\ 1,\ \gamma_L-\gamma_1-L\\ \gamma_L-\gamma_1+2,\ \gamma_L+\gamma_1-L+1\end{matrix};1\right)$$
$$-\frac{L(L+1)^2(\gamma_1+1)(L\gamma_1-L-1)}{(2L+1)(\gamma_{L+1}-\gamma_1+1)(\gamma_{L+1}+\gamma_1-L)}\,{}_3F_2\left(\begin{matrix}-L+1,\ 1,\ \gamma_{L+1}-\gamma_1-L\\ \gamma_{L+1}-\gamma_1+2,\ \gamma_{L+1}+\gamma_1-L+1\end{matrix};1\right)\Bigg\}. \tag{6.19}$$

At the first sight, it might seem that the constraint on Z, under which the above formula is valid, is the one in Eq. (6.14). This is indeed the case if $L \geqslant 2$, but for $L = 1$ the situation is different. A closer look at the left-hand side of Eq. (6.14) and at Eq. (3.27) shows that in the dipole case the convergence condition in the former equation is rooted in the presence of the constant terms in the Laguerre polynomials in the radial Sturmians $S_{n_r1}^{(0)}(r)$ and $T_{n_r1}^{(0)}(r)$. However, it is easy to show that the

TABLE IX. Exact analytical expressions for the static electric multipole nuclear shielding constants $\sigma_{EL\to EL}$ with $1 \leqslant L \leqslant 4$ for the Dirac one-electron atom in the ground state. The expressions have been derived from Eq. (6.19).

L	$\sigma_{EL\to EL}$	Constraint on Z
1	$\frac{1}{Z}$	$Z < \alpha^{-1}$
2	$\frac{1}{Z}\frac{104\gamma_1^2+110\gamma_1-79}{15(2\gamma_1+7)(4\gamma_1-1)}$	$Z < \alpha^{-1}\frac{\sqrt{15}}{4}$
3	$\frac{1}{Z}\frac{2064\gamma_1^4+14\,764\gamma_1^3+30\,968\gamma_1^2+7181\gamma_1-17\,177}{42(\gamma_1+7)(2\gamma_1+7)(4\gamma_1+11)(6\gamma_1-1)}$	$Z < \alpha^{-1}\frac{\sqrt{35}}{6}$
4	$\frac{1}{Z}\frac{14\,208\gamma_1^6+251\,184\gamma_1^5+1\,662\,556\gamma_1^4+4\,813\,404\gamma_1^3+5\,195\,413\gamma_1^2-862\,740\gamma_1-3\,136\,025}{90(\gamma_1+5)(\gamma_1+7)(2\gamma_1+5)(2\gamma_1+23)(4\gamma_1+11)(8\gamma_1-1)}$	$Z < \alpha^{-1}\frac{3\sqrt{7}}{8}$

series

$$\tilde{R}_1^{(-2,1)}(P^{(0)},Q^{(0)};P^{(0)},Q^{(0)}) = \sum_{n_r=-\infty}^{\infty}\frac{1}{\mu_{n_r1}^{(0)}-1}\int_0^\infty dr\,r^{-2}\big[P^{(0)}(r)\tilde{S}_{n_r1}^{(0)}(r)+Q^{(0)}(r)\tilde{T}_{n_r1}^{(0)}(r)\big]\int_0^\infty dr'\,r'\big[\mu_{n_r1}^{(0)}P^{(0)}(r')S_{n_r1}^{(0)}(r')+Q^{(0)}(r')T_{n_r1}^{(0)}(r')\big], \quad (6.20)$$

where

$$\tilde{S}_{n_r1}^{(0)}(r) = \sqrt{\frac{(1+\gamma_1)(|n_r|+2\gamma_1)|n_r|!}{2ZN_{n_r1}(N_{n_r1}-1)\Gamma(|n_r|+2\gamma_1)}}\left(\frac{2Zr}{a_0}\right)^{\gamma_1}e^{-Zr/a_0}\left[L_{|n_r|-1}^{(2\gamma_1)}(0)+\frac{1-N_{n_r1}}{|n_r|+2\gamma_1}L_{|n_r|}^{(2\gamma_1)}(0)\right] \quad (6.21a)$$

and

$$\tilde{T}_{n_r1}^{(0)}(r) = \sqrt{\frac{(1-\gamma_1)(|n_r|+2\gamma_1)|n_r|!}{2ZN_{n_r1}(N_{n_r1}-1)\Gamma(|n_r|+2\gamma_1)}}\left(\frac{2Zr}{a_0}\right)^{\gamma_1}e^{-Zr/a_0}\left[L_{|n_r|-1}^{(2\gamma_1)}(0)-\frac{1-N_{n_r1}}{|n_r|+2\gamma_1}L_{|n_r|}^{(2\gamma_1)}(0)\right], \quad (6.21b)$$

gives a null contribution to the integral $R_1^{(-2,1)}(P^{(0)},Q^{(0)};P^{(0)},Q^{(0)})$. In consequence, in the dipole case the limitation on Z is weaker than for higher multipoles, being simply the natural one $Z < \alpha^{-1}$. Hence, in summary, the constraint on the validity of the formula for $\sigma_{EL\to EL}$ displayed in Eq. (6.19) is

$$Z < \begin{cases}\alpha^{-1} & \text{for } L = 1,\\ \alpha^{-1}\frac{\sqrt{4L^2-1}}{2L} & \text{for } L \geqslant 2.\end{cases} \quad (6.22)$$

As it holds that $L \geqslant 1$, both ${}_3F_2(1)$ functions that appear in Eq. (6.19) are seen to be terminating ones. This implies that the susceptibilities of the sort considered here may be expressed in terms of elementary functions. Explicit formulas for $\sigma_{EL\to EL}$ with L constrained by $1 \leqslant L \leqslant 4$ are displayed in Table IX.

Since only elementary functions are involved, numerical values of $\sigma_{EL\to EL}$, if desired, may be computed to any required accuracy, even without having access to any specialized software. For this reason, we have decided not to provide tabulation of such data here.

To complete the task, we derive the quasirelativistic representations for the shielding constants $\sigma_{EL\to EL}$. Somewhat surprisingly, this appears to be a bit more involved than in the case of the three far-field susceptibilities analyzed in Secs. III to V. Referring to Eqs. (3.43) and (3.44), the quasirelativistic approximations for the two ${}_3F_2(1)$ functions in Eqs. (6.18a) and (6.18b) are found to be

$${}_3F_2\left(\begin{matrix}-L+1,\,1,\,\gamma_L-\gamma_1-L\\ \gamma_L-\gamma_1+2,\,\gamma_L+\gamma_1-L+1\end{matrix};1\right) \simeq \frac{3L+1}{2(L+1)}-(\alpha Z)^2\frac{L-1}{4L(L+1)}\left[\frac{L^2-5}{2(L+1)}+\frac{(L-1)(L-2)}{3(L+2)}\,{}_3F_2\left(\begin{matrix}-L+3,\,1,\,1\\ L+3,\,4\end{matrix};1\right)\right] \quad (6.23)$$

and

$${}_3F_2\left(\begin{matrix}-L+1,\,1,\,\gamma_{L+1}-\gamma_1-L\\ \gamma_{L+1}-\gamma_1+2,\,\gamma_{L+1}+\gamma_1-L+1\end{matrix};1\right) \simeq 1-(\alpha Z)^2\frac{L(L-1)}{6(L+1)(L+2)}\,{}_3F_2\left(\begin{matrix}-L+2,\,1,\,1\\ L+3,\,4\end{matrix};1\right), \quad (6.24)$$

respectively. It is seen that in both cases the coefficients at $(\alpha Z)^2$ involve the hypergeometric functions of the sort considered in Appendix E. From Eq. (E10), we obtain

$$ {}_3F_2\left(\begin{matrix}-L+2,\,1,\,1\\ L+3,\,4\end{matrix};1\right) = -\frac{3(L+2)(5L+4)}{2L(L+1)} + \frac{6(L+2)(2L+1)}{L(L-1)}[\psi(2L+1)-\psi(L+2)] \tag{6.25} $$

and

$$ {}_3F_2\left(\begin{matrix}-L+3,\,1,\,1\\ L+3,\,4\end{matrix};1\right) = -\frac{3(L+2)(5L+1)}{2L(L-1)} + \frac{6(L+2)(2L+1)}{(L-1)(L-2)}[\psi(2L)-\psi(L+2)] \tag{6.26} $$

(singularities at $L=1$ and $L=2$ in the above two equations are apparent only and are removable through the application of the L'Hospital rule), which allows us to rewrite Eqs. (6.23) and (6.24) as

$$ {}_3F_2\left(\begin{matrix}-L+1,\,1,\,\gamma_L-\gamma_1-L\\ \gamma_L-\gamma_1+2,\,\gamma_L+\gamma_1-L+1\end{matrix};1\right) \simeq \frac{3L+1}{2(L+1)} - (\alpha Z)^2\frac{(L-1)(2L+1)}{2L(L+1)}\left[\psi(2L+1)-\psi(L+1)-\frac{L+1}{2L+1}\right] \tag{6.27} $$

and

$$ {}_3F_2\left(\begin{matrix}-L+1,\,1,\,\gamma_{L+1}-\gamma_1-L\\ \gamma_{L+1}-\gamma_1+2,\,\gamma_{L+1}+\gamma_1-L+1\end{matrix};1\right) \simeq 1-(\alpha Z)^2\frac{2L+1}{L+1}\left[\psi(2L+1)-\psi(L+1)-\frac{L(5L+7)}{4(L+1)(2L+1)}\right], \tag{6.28} $$

respectively. Inserting the above two estimates into Eqs. (6.18a) and (6.18b) and passing to the quasirelativistic limit with the factors multiplying the two ${}_3F_2(1)$'s, one arrives at

$$ \sigma_{\mathrm{E}L\to\mathrm{E}L,L} \simeq \frac{2}{Z(L+1)(2L+1)}\left\{1-(\alpha Z)^2\frac{L-1}{L}\left[\psi(2L+1)-\psi(L+1)+\frac{6L^4+L^3+L^2-2L-2}{4L(L-1)(2L+1)}\right]\right\} \tag{6.29a} $$

and

$$ \sigma_{\mathrm{E}L\to\mathrm{E}L,-L-1} \simeq \frac{2}{ZL(2L+1)}\left\{1-(\alpha Z)^2\frac{L}{L+1}\left[\psi(2L+1)-\psi(L+1)-\frac{2L^2+7L+1}{4(2L+1)}\right]\right\}. \tag{6.29b} $$

Hence, we infer the following formula for the quasirelativistic approximations of the electric multipole shielding constants:

$$ \sigma_{\mathrm{E}L\to\mathrm{E}L} \simeq \frac{2}{ZL(L+1)}\left\{1-(\alpha Z)^2\frac{2L-1}{2L+1}\left[\psi(2L+1)-\psi(L+1)+\frac{L^3-2L^2+L-1}{2L(2L-1)}\right]\right\}. \tag{6.30} $$

Estimates of $\sigma_{\mathrm{E}L\to\mathrm{E}L}$ resulting from Eq. (6.30) are presented in Table X for $1 \leqslant L \leqslant 4$.

We have verified numerically that the quasirelativistic formula in Eq. (6.30) is equivalent to a much more complicated one given in Ref. [17, Eq. (37)], provided one corrects the latter and replaces $(2l-2)!$ with $(2l-n)!$. In addition, we remark that the quasirelativistic approximations to $\sigma_{\mathrm{E}L\to\mathrm{E}L}$ supplied in Refs. [26, Eq. (3)] and [16, Eq. (4.41)] are correct for $L=1$ and $L=3$, but for $L=2$ the factors k_2 and K_2 displayed therein should take the value $2/5$ instead of $59/150$.

TABLE X. Quasirelativistic approximations for static electric multipole shielding constants $\sigma_{\mathrm{E}L\to\mathrm{E}L}$ with $1 \leqslant L \leqslant 4$ for the Dirac one-electron atom in the ground state. The expressions have been derived from Eq. (6.27).

L	$\sigma_{\mathrm{E}L\to\mathrm{E}L}$
1	$\frac{1}{Z}$ (exact)
2	$\frac{1}{Z}\frac{1}{3}\left[1-\frac{2}{5}(\alpha Z)^2\right]$
3	$\frac{1}{Z}\frac{1}{6}\left[1-\frac{59}{84}(\alpha Z)^2\right]$
4	$\frac{1}{Z}\frac{1}{10}\left[1-\frac{529}{540}(\alpha Z)^2\right]$

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

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

Next we consider the near-nucleus magnetic multipole moments of the atom in the 2^L-pole electric field. In agreement with Eq. (B38), the spherical components of the 2^λ-pole moment of that sort are given by

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

where $\boldsymbol{j}(\boldsymbol{r})$ is the electronic current in the atom, defined as in Eq. (4.5). The same argument that has been applied to transform Eq. (4.1) into Eq. (4.4) allows us to rewrite the above definition as

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

Approximating the current as in Eq. (4.6) yields

$$\mathcal{N}_{\lambda\mu} \simeq \mathcal{N}^{(0)}_{\lambda\mu} + \mathcal{N}^{(1)}_{\lambda\mu}, \tag{7.3}$$

with

$$\mathcal{N}^{(0)}_{\lambda\mu} = -\frac{i}{\lambda}\sqrt{\frac{4\pi}{2\lambda+1}}\int_{\mathbb{R}^3} d^3\boldsymbol{r}\, r^{-\lambda-1} Y_{\lambda\mu}(\boldsymbol{n}_r)\boldsymbol{\Lambda}\cdot \boldsymbol{j}^{(0)}(\boldsymbol{r}) \tag{7.4}$$

and

$$\mathcal{N}^{(1)}_{\lambda\mu} = -\frac{i}{\lambda}\sqrt{\frac{4\pi}{2\lambda+1}}\int_{\mathbb{R}^3} d^3\boldsymbol{r}\, r^{-\lambda-1} Y_{\lambda\mu}(\boldsymbol{n}_r)\boldsymbol{\Lambda}\cdot \boldsymbol{j}^{(1)}(\boldsymbol{r}). \tag{7.5}$$

Evidently, angular integrations which arise when the integrals in Eqs. (7.4) and (7.5) are evaluated in the spherical coordinates are identical to these in Eqs. (4.10) and (4.11), respectively. This immediately allows us to write

$$\mathsf{N}_{\lambda} \simeq \mathsf{N}^{(0)}_{\lambda}\delta_{\lambda 1} + \mathsf{N}^{(1)}_{\lambda}(\delta_{\lambda,L-1} + \delta_{\lambda,L+1}), \tag{7.6}$$

where

$$\mathsf{N}^{(0)}_{1} = -\frac{4}{3}ec\boldsymbol{\nu}\int_0^\infty dr\, r^{-2} P^{(0)}(r) Q^{(0)}(r) \tag{7.7}$$

and

$$\mathsf{N}^{(1)}_{\lambda} = (4\pi\epsilon_0)c\frac{2\sqrt{2}(\lambda+1)}{(2\lambda+1)\sqrt{(2L+1)(\lambda+L+1)}} \times R^{(-\lambda-1,L)}_{\kappa_\lambda}(Q^{(0)},P^{(0)};P^{(0)},Q^{(0)})\{\boldsymbol{\nu}\otimes \mathsf{C}^{(1)}_L\}_\lambda \quad (\lambda = L\mp 1; \lambda\neq 0), \tag{7.8}$$

with κ_λ defined as in Eq. (4.34). We see that an isolated atom possesses only the permanent dipole moment of the sort considered, while the first-order moments of that kind induced by the 2^L-pole electric field are of ranks $L-1$ and $L+1$, except for the dipole ($L=1$) case when only the quadrupole moment arises [cf. Eq. (B42)].

Straightforward evaluation of the radial integral in Eq. (7.7) gives a closed-form representation of the permanent dipole moment $\mathsf{N}^{(0)}_1$,

$$\mathsf{N}^{(0)}_{1} = \frac{8}{3\gamma_1(2\gamma_1-1)}\frac{\mu_{\mathrm{B}}Z^3}{a_0^3}\boldsymbol{\nu} \quad \left(Z < \alpha^{-1}\frac{\sqrt{3}}{2}\right), \tag{7.9}$$

where the constraint on Z results from the convergence condition for the integral at its lower limit.

B. Atomic near-nucleus multipole EL → M($L \mp 1$) cross susceptibilities

The near-nucleus multipole electric-to-magnetic cross susceptibilities are defined through the relation

$$\mathsf{N}^{(1)}_{\lambda} = (4\pi\epsilon_0)c\sigma_{\mathrm{E}L\to\mathrm{M}\lambda}\frac{\{\boldsymbol{\nu}\otimes\mathsf{C}^{(1)}_L\}_\lambda}{\langle 10L0|\lambda 0\rangle} \quad (\lambda = L\mp 1; \lambda\neq 0), \tag{7.10}$$

where $\mathsf{N}^{(1)}_{\lambda}$ has been given in Eq. (7.8). Recalling the expression (4.36) for the Clebsch-Gordan coefficient $\langle 10L0|\lambda 0\rangle$ with $\lambda = L\mp 1$ yields the susceptibility $\sigma_{\mathrm{E}L\to\mathrm{M}\lambda}$ in the form

$$\sigma_{\mathrm{E}L\to\mathrm{M}\lambda} = \frac{2(\lambda+1)(\lambda-L)}{(2\lambda+1)(2L+1)}R^{(-\lambda-1,L)}_{\kappa_\lambda}(Q^{(0)},P^{(0)};P^{(0)},Q^{(0)}) \quad (\lambda = L\mp 1; \lambda\neq 0). \tag{7.11}$$

In view of Eqs. (3.15) and (3.26), we may write

$$R^{(-\lambda-1,L)}_{\kappa_\lambda}(Q^{(0)},P^{(0)};P^{(0)},Q^{(0)}) = \sum_{n_r=-\infty}^{\infty}\frac{1}{\mu^{(0)}_{n_r\kappa_\lambda}-1}\int_0^\infty dr\, r^{-\lambda-1}\big[Q^{(0)}(r)S^{(0)}_{n_r\kappa_\lambda}(r) + P^{(0)}(r)T^{(0)}_{n_r\kappa_\lambda}(r)\big] \times \int_0^\infty dr'\, r'^L\big[\mu^{(0)}_{n_r\kappa_\lambda}P^{(0)}(r')S^{(0)}_{n_r\kappa_\lambda}(r') + Q^{(0)}(r')T^{(0)}_{n_r\kappa_\lambda}(r')\big] \quad (\lambda = L\mp 1; \lambda\neq 0). \tag{7.12}$$

The second of the two integrals on the right-hand side of Eq. (7.12) is the same that has appeared in the last four sections, and its value has been given in Eq. (3.34). As regards the first one, its value may be deduced from Eq. (4.39), after the replacement $\lambda\to -\lambda-1$ is made in the latter, and this gives

$$\int_0^\infty dr\, r^{-\lambda-1}\big[Q^{(0)}(r)S^{(0)}_{n_r\kappa_\lambda}(r) + P^{(0)}(r)T^{(0)}_{n_r\kappa_\lambda}(r)\big] = -\alpha Z\left(\frac{2Z}{a_0}\right)^\lambda \frac{\sqrt{2}(N_{n_r\kappa_\lambda}-\kappa_\lambda)}{\sqrt{a_0|n_r|!N_{n_r\kappa_\lambda}(N_{n_r\kappa_\lambda}-\kappa_\lambda)\Gamma(2\gamma_1+1)\Gamma(|n_r|+2\gamma_{\kappa_\lambda}+1)}}\frac{\Gamma(\gamma_{\kappa_\lambda}+\gamma_1-\lambda)\Gamma(|n_r|+\gamma_{\kappa_\lambda}-\gamma_1+\lambda+1)}{\Gamma(\gamma_{\kappa_\lambda}-\gamma_1+\lambda+1)} \left[Z < \alpha^{-1}\frac{\sqrt{(2L+1)(2L+3)}}{2(L+1)} \text{ for } \lambda = L+1\right], \tag{7.13}$$

where the constraint, henceforth tacitly assumed to hold, guarantees that the integral in question converges at its lower limit. Plugging Eqs. (3.34) and (7.13) into Eq. (7.12), and then the latter into Eq. (7.11), after transformations which are already routine

TABLE XI. Exact analytical expressions for the near-nucleus static electric-to-magnetic multipole cross susceptibilities of the Dirac one-electron atom in the ground state. The expressions for $\sigma_{\mathrm{E}L\to\mathrm{M}(L-1)}$ with $2 \leqslant L \leqslant 4$, derived from Eq. (7.16) 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 $\sigma_{\mathrm{E}L\to\mathrm{M}(L+1)}$ with $1 \leqslant L \leqslant 4$, obtained from Eq. (7.17) and given in the third column, remain valid.

L	$\sigma_{\mathrm{E}L\to\mathrm{M}(L-1)}$	$\sigma_{\mathrm{E}L\to\mathrm{M}(L+1)}$	Constraint on Z in $\sigma_{\mathrm{E}L\to\mathrm{M}(L+1)}$
1		$-\frac{\alpha Z}{a_0}\frac{6(3\gamma_1+1)}{5\gamma_1(\gamma_1+1)(4\gamma_1-1)}$	$Z < \alpha^{-1}\frac{\sqrt{15}}{4}$
2	$-\frac{\alpha a_0}{Z}\frac{2\gamma_1+1}{9}$	$\frac{\alpha Z}{a_0}\frac{16(6\gamma_1^3-\gamma_1^2-36\gamma_1-14)}{35\gamma_1(\gamma_1+1)(2\gamma_1+7)(6\gamma_1-1)}$	$Z < \alpha^{-1}\frac{\sqrt{35}}{6}$
3	$-\frac{\alpha a_0}{Z}\frac{3(2\gamma_1+1)(2\gamma_1+5)}{28(2\gamma_1+7)}$	$\frac{\alpha Z}{a_0}\frac{50(32\gamma_1^4+164\gamma_1^3-53\gamma_1^2-584\gamma_1-231)}{189\gamma_1(\gamma_1+1)(\gamma_1+7)(4\gamma_1+11)(8\gamma_1-1)}$	$Z < \alpha^{-1}\frac{3\sqrt{7}}{8}$
4	$-\frac{\alpha a_0}{Z}\frac{2(2\gamma_1+1)(68\gamma_1^2+483\gamma_1+709)}{315(\gamma_1+7)(4\gamma_1+11)}$	$\frac{\alpha Z}{a_0}\frac{2(60\gamma_1^5+744\gamma_1^4+2065\gamma_1^3-964\gamma_1^2-5905\gamma_1-2300)}{11\gamma_1(\gamma_1+1)(\gamma_1+5)(2\gamma_1+5)(2\gamma_1+23)(10\gamma_1-1)}$	$Z < \alpha^{-1}\frac{3\sqrt{11}}{10}$

at this stage, we obtain

$$\begin{aligned}\sigma_{\mathrm{E}L\to\mathrm{M}\lambda} = {} & \frac{\alpha a_0^{L-\lambda}}{Z^{L-\lambda}}\frac{(\lambda+1)(\lambda-L)\Gamma(2\gamma_1-\lambda+L+1)}{2^{L-\lambda-1}(\kappa_\lambda+1)(2\lambda+1)(2L+1)\Gamma(2\gamma_1+1)} \\ & \times\left\{1+\frac{\lambda[\gamma_1(\kappa_\lambda+1)+L+1]\Gamma(\gamma_{\kappa_\lambda}+\gamma_1-\lambda)\Gamma(\gamma_{\kappa_\lambda}+\gamma_1+L+1)}{(\gamma_{\kappa_\lambda}-\gamma_1+1)\Gamma(2\gamma_1-\lambda+L+1)\Gamma(2\gamma_{\kappa_\lambda}+1)}\right. \\ & \left.\times\,{}_3F_2\left(\begin{matrix}\gamma_{\kappa_\lambda}-\gamma_1+\lambda+1,\ \gamma_{\kappa_\lambda}-\gamma_1-L,\ \gamma_{\kappa_\lambda}-\gamma_1+1\\ \gamma_{\kappa_\lambda}-\gamma_1+2,\ 2\gamma_{\kappa_\lambda}+1\end{matrix};1\right)\right\} \quad (\lambda = L\mp 1;\ \lambda\neq 0).\end{aligned} \tag{7.14}$$

Applying the identity (6.16) to the hypergeometric function of the right-hand side of Eq. (7.14) casts the latter formula to the simpler form

$$\begin{aligned}\sigma_{\mathrm{E}L\to\mathrm{M}\lambda} = {} & \frac{\alpha a_0^{L-\lambda}}{Z^{L-\lambda}}\frac{(\lambda+1)(\lambda-L)\Gamma(2\gamma_1-\lambda+L+1)}{2^{L-\lambda-1}(\kappa_\lambda+1)(2\lambda+1)(2L+1)\Gamma(2\gamma_1+1)} \\ & \times\left\{1+\frac{\lambda[\gamma_1(\kappa_\lambda+1)+L+1]}{(\gamma_{\kappa_\lambda}-\gamma_1+1)(\gamma_{\kappa_\lambda}+\gamma_1-\lambda)}\,{}_3F_2\left(\begin{matrix}-\lambda+1,\ 1,\ \gamma_{\kappa_\lambda}-\gamma_1-L\\ \gamma_{\kappa_\lambda}-\gamma_1+2,\ \gamma_{\kappa_\lambda}+\gamma_1-\lambda+1\end{matrix};1\right)\right\} \quad (\lambda = L\mp 1;\ \lambda\neq 0),\end{aligned} \tag{7.15}$$

where the ${}_3F_2(1)$ function is a truncating one. Hence, we find that the explicit representations of the two cross susceptibilities $\sigma_{\mathrm{E}L\to\mathrm{M}(L\mp1)}$ are

$$\begin{aligned}\sigma_{\mathrm{E}L\to\mathrm{M}(L-1)} = {} & -\frac{\alpha a_0}{Z}\frac{L(2\gamma_1+1)}{(L+1)(4L^2-1)}\left\{1+\frac{(L^2-1)(\gamma_1+1)}{(\gamma_L-\gamma_1+1)(\gamma_L+\gamma_1-L+1)}\,{}_3F_2\left(\begin{matrix}-L+2,\ 1,\ \gamma_L-\gamma_1-L\\ \gamma_L-\gamma_1+2,\ \gamma_L+\gamma_1-L+2\end{matrix};1\right)\right\} \\ & (L\neq 1)\end{aligned} \tag{7.16}$$

and

$$\begin{aligned}\sigma_{\mathrm{E}L\to\mathrm{M}(L+1)} = {} & -\frac{\alpha Z}{a_0}\frac{2(L+2)}{\gamma_1 L(2L+1)(2L+3)}\left\{1-\frac{(L+1)(L\gamma_1-L-1)}{(\gamma_{L+1}-\gamma_1+1)(\gamma_{L+1}+\gamma_1-L-1)}\,{}_3F_2\left(\begin{matrix}-L,\ 1,\ \gamma_{L+1}-\gamma_1-L\\ \gamma_{L+1}-\gamma_1+2,\ \gamma_{L+1}+\gamma_1-L\end{matrix};1\right)\right\} \\ & \left[Z<\alpha^{-1}\frac{\sqrt{(2L+1)(2L+3)}}{2(L+1)}\right].\end{aligned} \tag{7.17}$$

Elementary expressions for $\sigma_{\mathrm{E}L\to\mathrm{M}(L-1)}$ with $2 \leqslant L \leqslant 4$ and $\sigma_{\mathrm{E}L\to\mathrm{M}(L+1)}$ with $1 \leqslant L \leqslant 4$, inferred from Eqs. (7.16) and (7.17), are displayed in Table XI.

To establish the quasirelativistic approximations to the formulas in Eqs. (7.16) and (7.17), we consider the estimates

$$\begin{aligned}& {}_3F_2\left(\begin{matrix}-L+2,\ 1,\ \gamma_L-\gamma_1-L\\ \gamma_L-\gamma_1+2,\ \gamma_L+\gamma_1-L+2\end{matrix};1\right) \\ & \simeq \frac{4L+1}{3(L+1)}-(\alpha Z)^2\frac{L-2}{6L(L+1)}\left[\frac{2L^2+L-7}{3(L+1)}+\frac{(L-1)(L-3)}{4(L+2)}\,{}_3F_2\left(\begin{matrix}-L+4,\ 1,\ 1\\ L+3,\ 5\end{matrix};1\right)\right]\end{aligned} \tag{7.18}$$

and

$$ {}_3F_2\left(\begin{matrix}-L,\,1,\,\gamma_{L+1}-\gamma_1-L\\ \gamma_{L+1}-\gamma_1+2,\,\gamma_{L+1}+\gamma_1-L\end{matrix};1\right)\simeq 1-(\alpha Z)^2\frac{L^2}{4(L+1)(L+2)}\,{}_3F_2\left(\begin{matrix}-L+1,\,1,\,1\\ L+3,\,3\end{matrix};1\right), \tag{7.19}$$

which, with the aid of the identities

$$ {}_3F_2\left(\begin{matrix}-L+4,\,1,\,1\\ L+3,\,5\end{matrix};1\right)=\frac{8(L+2)(4L^2-1)}{(L-1)(L-2)(L-3)}[\psi(2L+1)-\psi(L+2)]-\frac{2(L+2)(32L-19)}{3(L-2)(L-3)} \tag{7.20}$$

[cf. Eq. (E11)] and

$$ {}_3F_2\left(\begin{matrix}-L+1,\,1,\,1\\ L+3,\,3\end{matrix};1\right)=\frac{4(L+2)}{L}[\psi(2L+2)-\psi(L+2)]-\frac{2(L+2)}{L+1} \tag{7.21}$$

[cf. Eq. (E3)], may be rewritten as

$$ {}_3F_2\left(\begin{matrix}-L+2,\,1,\,\gamma_L-\gamma_1-L\\ \gamma_L-\gamma_1+2,\,\gamma_L+\gamma_1-L+2\end{matrix};1\right)\simeq\frac{4L+1}{3(L+1)}-(\alpha Z)^2\frac{4L^2-1}{3L(L+1)}\left[\psi(2L+1)-\psi(L+1)-\frac{7(L+1)(4L-3)}{12(4L^2-1)}\right] \tag{7.22}$$

and

$$ {}_3F_2\left(\begin{matrix}-L,\,1,\,\gamma_{L+1}-\gamma_1-L\\ \gamma_{L+1}-\gamma_1+2,\,\gamma_{L+1}+\gamma_1-L\end{matrix};1\right)\simeq 1-(\alpha Z)^2\frac{L}{L+1}\left[\psi(2L+2)-\psi(L+2)-\frac{L}{2(L+1)}\right], \tag{7.23}$$

respectively. Applying the estimates in Eqs. (3.43), (7.22), and (7.23) to the right-hand sides of Eqs. (7.16) and (7.17), after some algebra we arrive at the sought quasirelativistic approximations

$$\sigma_{\mathrm{E}L\to\mathrm{M}(L-1)}\simeq-\frac{\alpha a_0}{Z}\frac{1}{L+1}\left\{1-(\alpha Z)^2\frac{L-1}{L}\left[\psi(2L)-\psi(L)-\frac{L(4L^2-3L-5)}{4(L-1)(4L^2-1)}\right]\right\}\quad(L\neq 1) \tag{7.24}$$

and

$$\sigma_{\mathrm{E}L\to\mathrm{M}(L+1)}\simeq-\frac{\alpha Z}{a_0}\frac{4(L+2)}{L(2L+1)(2L+3)}\left\{1-(\alpha Z)^2\frac{L}{2(L+1)}\left[\psi(2L+2)-\psi(L+1)-\frac{(L+1)(L+4)}{2L}\right]\right\}. \tag{7.25}$$

Particular cases of the later two formulas are displayed in Table XII.

VIII. NEAR-NUCLEUS MAGNETIC TOROIDAL MULTIPOLE MOMENTS OF THE ATOM IN THE MULTIPOLE ELECTRIC FIELD AND NEAR-NUCLEUS EL → TL MULTIPOLE CROSS SUSCEPTIBILITIES

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

The last family of the atomic multipole moments we wish to look at in the present work are the near-nucleus magnetic toroidal multipole moments U_λ. According to Eq. (D10), their spherical components may be defined as

$$\mathcal{U}_{\lambda\mu}=-\frac{1}{\lambda}\sqrt{\frac{4\pi}{2\lambda+1}}\int_{\mathbb{R}^3}d^3\boldsymbol{r}\,r^{-\lambda-1}Y_{\lambda\mu}(\boldsymbol{n}_r)\boldsymbol{r}\cdot\boldsymbol{j}(\boldsymbol{r}). \tag{8.1}$$

In the weak-perturbing-field regime, which we consider in this paper, after exploiting Eq. (4.6), we have

$$\mathcal{U}_{\lambda\mu}\simeq\mathcal{U}^{(0)}_{\lambda\mu}+\mathcal{U}^{(1)}_{\lambda\mu}, \tag{8.2}$$

with

$$\mathcal{U}^{(0)}_{\lambda\mu}=-\frac{1}{\lambda}\sqrt{\frac{4\pi}{2\lambda+1}}\int_{\mathbb{R}^3}d^3\boldsymbol{r}\,r^{-\lambda-1}Y_{\lambda\mu}(\boldsymbol{n}_r)\boldsymbol{r}\cdot\boldsymbol{j}^{(0)}(\boldsymbol{r}) \tag{8.3}$$

and

$$\mathcal{U}^{(1)}_{\lambda\mu}=-\frac{1}{\lambda}\sqrt{\frac{4\pi}{2\lambda+1}}\int_{\mathbb{R}^3}d^3\boldsymbol{r}\,r^{-\lambda-1}Y_{\lambda\mu}(\boldsymbol{n}_r)\boldsymbol{r}\cdot\boldsymbol{j}^{(1)}(\boldsymbol{r}) \tag{8.4}$$

being the permanent and the first-order induced parts, respectively, of the moment under study in the atomic ground state. Exactly in the same manner as in Sec. V, one may show that the isolated atom in the ground state does not possess any nonvanishing moments of the sort considered,

$$\mathsf{U}^{(0)}_\lambda=0, \tag{8.5}$$

TABLE XII. Quasirelativistic approximations for the near-nucleus static electric-to-magnetic multipole cross susceptibilities $\sigma_{\mathrm{E}L\to\mathrm{M}(L-1)}$ with $2\leqslant L\leqslant 4$ and $\sigma_{\mathrm{E}L\to\mathrm{M}(L+1)}$ with $1\leqslant L\leqslant 4$ for the Dirac one-electron atom in the ground state. The expressions have been derived from Eqs. (7.24) and (7.25).

L	$\sigma_{\mathrm{E}L\to\mathrm{M}(L-1)}$	$\sigma_{\mathrm{E}L\to\mathrm{M}(L+1)}$
1		$-\frac{\alpha a_0}{Z}\frac{4}{5}\left[1+\frac{25}{24}(\alpha Z)^2\right]$
2	$-\frac{\alpha Z}{a_0}\frac{1}{3}\left[1-\frac{1}{3}(\alpha Z)^2\right]$	$-\frac{\alpha a_0}{Z}\frac{8}{35}\left[1+\frac{223}{180}(\alpha Z)^2\right]$
3	$-\frac{\alpha Z}{a_0}\frac{1}{4}\left[1-\frac{23}{63}(\alpha Z)^2\right]$	$-\frac{\alpha a_0}{Z}\frac{20}{189}\left[1+\frac{1641}{1120}(\alpha Z)^2\right]$
4	$-\frac{\alpha Z}{a_0}\frac{1}{5}\left[1-\frac{1931}{5040}(\alpha Z)^2\right]$	$-\frac{\alpha a_0}{Z}\frac{2}{33}\left[1+\frac{10\,721}{6300}(\alpha Z)^2\right]$

and that the only induced moment is the one with the multipolar symmetry identical to that of the perturbing electric field, i.e.,

$$\mathsf{U}_\lambda \simeq \mathsf{U}_\lambda^{(1)}\delta_{\lambda L}, \tag{8.6}$$

with

$$\mathsf{U}_L^{(1)} = (4\pi\epsilon_0)c\,\frac{2i}{(2L+1)^2}\sqrt{\frac{L+1}{L}}\left[R_L^{(-L,L)}(Q^{(0)},-P^{(0)};P^{(0)},Q^{(0)}) - R_{-L-1}^{(-L,L)}(Q^{(0)},-P^{(0)};P^{(0)},Q^{(0)})\right]\left\{\boldsymbol{\nu}\otimes\mathsf{C}_L^{(1)}\right\}_L \tag{8.7}$$

[for the definition of the double radial integrals $R_\kappa^{(-L,L)}(Q^{(0)},-P^{(0)};P^{(0)},Q^{(0)})$, see Eq. (3.15)].

B. Atomic near-nucleus multipole E$L \to$ TL cross susceptibilities

In complete analogy to the far-field case discussed in Sec. V B, we define the near-nucleus multipole E$L \to$ TL cross susceptibilities through the relation

$$\mathsf{U}_L^{(1)} = i(4\pi\epsilon_0)c\sigma_{\mathrm{E}L\to\mathrm{T}L}\sqrt{L(L+1)}\left\{\boldsymbol{\nu}\otimes\mathsf{C}_L^{(1)}\right\}_L. \tag{8.8}$$

Comparison of Eqs. (8.7) and (8.8) yields $\sigma_{\mathrm{E}L\to\mathrm{T}L}$ as the sum

$$\sigma_{\mathrm{E}L\to\mathrm{T}L} = \sigma_{\mathrm{E}L\to\mathrm{T}L,L} + \sigma_{\mathrm{E}L\to\mathrm{T}L,-L-1}, \tag{8.9}$$

where

$$\sigma_{\mathrm{E}L\to\mathrm{T}L,\kappa} = \frac{2\,\mathrm{sgn}(\kappa)}{L(2L+1)^2}R_\kappa^{(-L,L)}(Q^{(0)},-P^{(0)};P^{(0)},Q^{(0)}) \quad (\kappa = L,-L-1). \tag{8.10}$$

After the Sturmian expansion (3.26) is used, the double radial integral appearing in Eq. (8.10) takes the form of the series

$$R_\kappa^{(-L,L)}(Q^{(0)},-P^{(0)};P^{(0)},Q^{(0)}) = \sum_{n_r=-\infty}^{\infty}\frac{1}{\mu_{n_r\kappa}^{(0)}-1}\int_0^\infty dr\,r^{-L}\left[Q^{(0)}(r)S_{n_r\kappa}^{(0)}(r) - P^{(0)}(r)T_{n_r\kappa}^{(0)}(r)\right]$$
$$\times\int_0^\infty dr'\,r'^L\left[\mu_{n_r\kappa}^{(0)}P^{(0)}(r')S_{n_r\kappa}^{(0)}(r') + Q^{(0)}(r')T_{n_r\kappa}^{(0)}(r')\right]. \tag{8.11}$$

With no difficulty, from Eqs. (2.11), (3.27), and (3.31) one finds that

$$\int_0^\infty dr\,r^{-L}\left[Q^{(0)}(r)S_{n_r\kappa}^{(0)}(r) - P^{(0)}(r)T_{n_r\kappa}^{(0)}(r)\right]$$
$$= \alpha Z\left(\frac{2Z}{a_0}\right)^{L-1}\frac{\sqrt{2}\,|n_r|(|n_r|+2\gamma_\kappa)}{\sqrt{a_0|n_r|!N_{n_r\kappa}(N_{n_r\kappa}-\kappa)\Gamma(2\gamma_1+1)\Gamma(|n_r|+2\gamma_\kappa+1)}}\frac{\Gamma(\gamma_\kappa+\gamma_1-L+1)\Gamma(|n_r|+\gamma_\kappa-\gamma_1+L-1)}{\Gamma(\gamma_\kappa-\gamma_1+L)}. \tag{8.12}$$

Inserting Eqs. (3.28), (3.34), and (8.12) into Eq. (8.11) and proceeding then along the same path as in the preceding sections to transform the series $\sum_{n_r=-\infty}^{\infty}(\cdots)$ into the one of the form $\sum_{n_r=0}^{\infty}(\cdots)$, we arrive at

$$\sigma_{\mathrm{E}L\to\mathrm{T}L,\kappa} = -\frac{\alpha a_0}{Z}\frac{\mathrm{sgn}(\kappa)[\gamma_1(\kappa+1)+L+1]\Gamma(\gamma_\kappa+\gamma_1-L+1)\Gamma(\gamma_\kappa+\gamma_1+L+1)}{L(2L+1)^2(\gamma_\kappa-\gamma_1+1)\Gamma(2\gamma_1+1)\Gamma(2\gamma_\kappa+1)}$$
$$\times\,{}_3F_2\left(\begin{matrix}\gamma_\kappa-\gamma_1+L,\ \gamma_\kappa-\gamma_1-L,\ \gamma_\kappa-\gamma_1+1\\ \gamma_\kappa-\gamma_1+2,\ 2\gamma_\kappa+1\end{matrix};1\right) \quad (\kappa = L,-L-1). \tag{8.13}$$

In the final step, we apply the hypergeometric identity (6.16) to convert the ${}_3F_2(1)$ series in Eq. (8.13) into a more suitable one, which yields

$$\sigma_{\mathrm{E}L\to\mathrm{T}L,\kappa} = -\frac{\alpha a_0}{Z}\frac{\mathrm{sgn}(\kappa)(2\gamma_1+1)[\gamma_1(\kappa+1)+L+1]}{L(2L+1)^2(\gamma_\kappa-\gamma_1+1)(\gamma_\kappa+\gamma_1-L+1)}$$
$$\times\,{}_3F_2\left(\begin{matrix}-L+2,\ 1,\ \gamma_\kappa-\gamma_1-L\\ \gamma_\kappa-\gamma_1+2,\ \gamma_\kappa+\gamma_1-L+2\end{matrix};1\right) \quad (\kappa = L,-L-1). \tag{8.14}$$

Hence, the cross susceptibility $\sigma_{\mathrm{E}L\to\mathrm{T}L}$ is the sum of

$$\sigma_{\mathrm{E}L\to\mathrm{T}L,L} = -\frac{\alpha a_0}{Z}\frac{(L+1)(\gamma_1+1)(2\gamma_1+1)}{L(2L+1)^2(\gamma_L-\gamma_1+1)(\gamma_L+\gamma_1-L+1)}\,{}_3F_2\left(\begin{matrix}-L+2,\ 1,\ \gamma_L-\gamma_1-L\\ \gamma_L-\gamma_1+2,\ \gamma_L+\gamma_1-L+2\end{matrix};1\right) \tag{8.15a}$$

and

$$\sigma_{\mathrm{E}L\to\mathrm{T}L,-L-1} = -\frac{\alpha a_0}{Z}\frac{(2\gamma_1+1)(L\gamma_1-L-1)}{L(2L+1)^2(\gamma_{L+1}-\gamma_1+1)(\gamma_{L+1}+\gamma_1-L+1)}\,{}_3F_2\left(\begin{matrix}-L+2,\ 1,\ \gamma_{L+1}-\gamma_1-L\\ \gamma_{L+1}-\gamma_1+2,\ \gamma_{L+1}+\gamma_1-L+2\end{matrix};1\right) \tag{8.15b}$$

TABLE XIII. Exact analytical expressions for the near-nucleus static electric-to-magnetic-toroidal multipole cross susceptibilities $\sigma_{\mathrm{E}L\to\mathrm{T}L}$ with $1 \leqslant L \leqslant 4$ for the Dirac one-electron atom in the ground state. The formulas have been derived from Eq. (8.16) and are valid under the constraint $Z < \alpha^{-1}$.

L	$\sigma_{\mathrm{E}L\to\mathrm{T}L}$
1	$-\frac{\alpha a_0}{Z}\frac{1}{9}\left[\frac{(\gamma_1+1)(4\gamma_1+1)}{2\gamma_1}+\frac{(\gamma_1-2)(2\gamma_1+1)}{\gamma_2+\gamma_1+3}\,{}_3F_2\left(\begin{matrix}1,\,1,\,\gamma_2-\gamma_1-1\\ \gamma_2-\gamma_1+2,\,\gamma_2+\gamma_1+1\end{matrix};1\right)\right]$
2	$-\frac{\alpha a_0}{Z}\frac{(2\gamma_1+1)(2\gamma_1+3)}{20(2\gamma_1+7)}$
3	$-\frac{\alpha a_0}{Z}\frac{(\gamma_1+1)(2\gamma_1+1)(4\gamma_1^2+34\gamma_1+67)}{21(\gamma_1+7)(2\gamma_1+7)(4\gamma_1+11)}$
4	$-\frac{\alpha a_0}{Z}\frac{(2\gamma_1+1)(48\gamma_1^5+1092\gamma_1^4+8856\gamma_1^3+31\,625\gamma_1^2+48\,384\gamma_1+23\,395)}{216(\gamma_1+5)(\gamma_1+7)(2\gamma_1+5)(2\gamma_1+23)(4\gamma_1+11)}$

and is explicitly given by

$$\sigma_{\mathrm{E}L\to\mathrm{T}L} = -\frac{\alpha a_0}{Z}\frac{(L+1)(2\gamma_1+1)}{L(2L+1)^2}\left\{\frac{\gamma_1+1}{(\gamma_L-\gamma_1+1)(\gamma_L+\gamma_1-L+1)}\,{}_3F_2\left(\begin{matrix}-L+2,\,1,\,\gamma_L-\gamma_1-L\\ \gamma_L-\gamma_1+2,\,\gamma_L+\gamma_1-L+2\end{matrix};1\right)\right.$$
$$\left.+\frac{L\gamma_1-L-1}{(L+1)(\gamma_{L+1}-\gamma_1+1)(\gamma_{L+1}+\gamma_1-L+1)}\,{}_3F_2\left(\begin{matrix}-L+2,\,1,\,\gamma_{L+1}-\gamma_1-L\\ \gamma_{L+1}-\gamma_1+2,\,\gamma_{L+1}+\gamma_1-L+2\end{matrix};1\right)\right\}. \tag{8.16}$$

For $L \geqslant 2$, both hypergeometric series on the right-hand side of Eq. (8.16) truncate, and consequently the corresponding cross susceptibilities $\sigma_{\mathrm{E}L\to\mathrm{T}L}$ may be written in terms of elementary functions. The dipole ($L = 1$) case is different since then the second ${}_3F_2(1)$ function remains transcendental. Explicit analytical expressions for the cross susceptibilities $\sigma_{\mathrm{E}L\to\mathrm{T}L}$ with $1 \leqslant L \leqslant 4$ are presented in Table XIII. In turn, in Table XIV we provide numerical data for the dipole cross susceptibility $\sigma_{\mathrm{E}1\to\mathrm{T}1}$ for selected values of the nuclear charge number Z.

We move to the derivation of the quasirelativistic limit of the expression in Eq. (8.16). The ${}_3F_2(1)$ function in Eq. (8.15a) is the one we have already come across in Sec. VII B, and the approximation to it is given in Eq. (7.22). In turn, for the hypergeometric function in Eq. (8.15b) we have

$${}_3F_2\left(\begin{matrix}-L+2,\,1,\,\gamma_{L+1}-\gamma_1-L\\ \gamma_{L+1}-\gamma_1+2,\,\gamma_{L+1}+\gamma_1-L+2\end{matrix};1\right) \simeq 1-(\alpha Z)^2\frac{L(L-2)}{8(L+1)(L+2)}\,{}_3F_2\left(\begin{matrix}-L+3,\,1,\,1\\ L+3,\,5\end{matrix};1\right). \tag{8.17}$$

From Eq. (E11) we have

$${}_3F_2\left(\begin{matrix}-L+3,\,1,\,1\\ L+3,\,5\end{matrix};1\right) = \frac{16(L+2)(2L+1)}{(L-1)(L-2)}[\psi(2L)-\psi(L+2)] - \frac{4(L+2)(16L^2+17L+3)}{3L(L^2-1)} \tag{8.18}$$

(we do not exclude the cases $L = 1$ and $L = 2$ as singularities at these two values of L in the expression on the right-hand side are only apparent and are removable via the passage to the limit procedure) and consequently the ${}_3F_2(1)$ function in Eq. (8.15b) may be approximated as

$${}_3F_2\left(\begin{matrix}-L+2,\,1,\,\gamma_{L+1}-\gamma_1-L\\ \gamma_{L+1}-\gamma_1+2,\,\gamma_{L+1}+\gamma_1-L+2\end{matrix};1\right) \simeq 1-(\alpha Z)^2\frac{2L(2L+1)}{L^2-1}\left[\psi(2L+1)-\psi(L+1)-\frac{16L^2+21L-1}{12(L+1)(2L+1)}\right]. \tag{8.19}$$

Using Eqs. (7.22) and (8.19), after some algebraic simplifications we obtain

$$\sigma_{\mathrm{E}L\to\mathrm{T}L,L} \simeq -\frac{\alpha a_0}{Z}\frac{4L+1}{L^2(2L+1)^2}\left\{1-(\alpha Z)^2\frac{4L^2-1}{L(4L+1)}\left[\psi(2L-1)-\psi(L)-\frac{4L^2-3L-4}{4(4L^2-1)}\right]\right\} \tag{8.20a}$$

and

$$\sigma_{\mathrm{E}L\to\mathrm{T}L,-L-1} \simeq \frac{\alpha a_0}{Z}\frac{1}{L(L+1)(2L+1)^2}\left\{1-(\alpha Z)^2\frac{2L(2L+1)}{L^2-1}\left[\psi(2L+1)-\psi(L+1)-\frac{L(L+5)}{4(2L+1)}\right]\right\}. \tag{8.20b}$$

Hence, the sought approximate expression for the cross susceptibility $\sigma_{\mathrm{E}L\to\mathrm{T}L}$ is

$$\sigma_{\mathrm{E}L\to\mathrm{T}L} \simeq -\frac{\alpha a_0}{Z}\frac{1}{L^2(L+1)}\left\{1-(\alpha Z)^2\frac{2L^4-L^3-3L^2-L+1}{L(2L+1)(L^2-1)}\left[\psi(2L)-\psi(L)-\frac{L(L^3-L^2-3L-5)}{4(2L^4-L^3-3L^2-L+1)}\right]\right\}. \tag{8.21}$$

TABLE XIV. The near-nucleus static electric-to-toroidal-magnetic dipole cross susceptibilities $\sigma_{\mathrm{E1}\to\mathrm{T1}}$ for selected hydrogenic ions in the ground state, computed from Eq. (8.16) with $L = 1$. 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	$\sigma_{\mathrm{E1}\to\mathrm{T1}}$ (units of a_0)
1	$-3.648\,637\,095\,60\,(83) \times 10^{-3}$
2	$-1.824\,259\,765\,87\,(41) \times 10^{-3}$
5	$-7.295\,393\,076\,3\,(17) \times 10^{-4}$
10	$-3.644\,756\,614\,28\,(82) \times 10^{-4}$
20	$-1.816\,493\,443\,61\,(41) \times 10^{-4}$
40	$-8.964\,422\,142\,8\,(20) \times 10^{-5}$
60	$-5.844\,669\,492\,5\,(13) \times 10^{-5}$
80	$-4.246\,284\,894\,89\,(82) \times 10^{-5}$
100	$-3.264\,717\,305\,27\,(59) \times 10^{-5}$
120	$-2.646\,549\,207\,67\,(64) \times 10^{-5}$
137	$-1.413\,712\,75\,(56) \times 10^{-4}$

In the particular case of $L = 1$, after the L'Hospital rule is applied (this is admissible since L may be formally treated as a continuous parameter; cf. Appendix E) and the well-known identities

$$\psi'(1) = \frac{\pi^2}{6}, \quad \psi'(2) = \frac{\pi^2}{6} - 1, \tag{8.22}$$

are exploited, Eq. (8.21) becomes

$$\sigma_{\mathrm{E1}\to\mathrm{T1}} \simeq -\frac{\alpha a_0}{Z}\frac{1}{2}\left[1 - \left(\frac{3}{4} - \frac{\pi^2}{18}\right)(\alpha Z)^2\right]. \tag{8.23}$$

The explicit forms of the quasirelativistic approximations to $\sigma_{\mathrm{E}L\to\mathrm{T}L}$ for $1 \leqslant L \leqslant 4$, resulting from Eqs. (8.23) and (8.21), are displayed in Table XV.

IX. SUMMARY AND FUTURE PROSPECTIVES

In this paper, we have considered various far- and near-field electric and magnetic multipole moments induced in the ground state of the Dirac one-electron atom by an external, weak, static electric 2^L-pole field. Strengths of all these induced moments have been characterized by congruent atomic multipole susceptibilities, using formulas brought together in Table XVI. Table XVII shows how the susceptibilities in question enter the near- and far-zone asymptotic representations of the lowest-order electric and magnetic fields and their potentials, generated by the atom in response to the perturbation. For the reader's convenience, all exact closed-form analytical expressions for the susceptibilities, derived by us in Secs. III–VIII with the aid of the Sturmian expansion of the Dirac-Coulomb Green function, are collected in Tables XVIII and XIX.

TABLE XV. Quasirelativistic approximations for the near-nucleus static electric-to-toroidal-magnetic multipole cross susceptibilities $\sigma_{\mathrm{E}L\to\mathrm{T}L}$ with $1 \leqslant L \leqslant 4$ for the Dirac one-electron atom in the ground state. The expression for $L = 1$ is the one displayed in Eq. (8.23), while these for $2 \leqslant L \leqslant 4$ have been derived from Eq. (8.21).

L	$\sigma_{\mathrm{E}L\to\mathrm{T}L}$
1	$-\frac{\alpha a_0}{Z}\frac{1}{2}\left[1 - \left(\frac{3}{4} - \frac{\pi^2}{18}\right)(\alpha Z)^2\right]$
2	$-\frac{\alpha a_0}{Z}\frac{1}{12}\left[1 - \frac{19}{45}(\alpha Z)^2\right]$
3	$-\frac{\alpha a_0}{Z}\frac{1}{36}\left[1 - \frac{343}{720}(\alpha Z)^2\right]$
4	$-\frac{\alpha a_0}{Z}\frac{1}{80}\left[1 - \frac{113\,623}{226\,800}(\alpha Z)^2\right]$

In Tables II, IV, V, and VII, embedded in Secs. III–V, we have provided numerical values of the far-field susceptibilities α_L ($\equiv \alpha_{\mathrm{E}L\to\mathrm{E}L}$), $\alpha_{\mathrm{E}L\to\mathrm{M}(L\mp1)}$, and $\alpha_{\mathrm{E}L\to\mathrm{T}L}$, all with $1 \leqslant L \leqslant 4$, only for some representative nuclear charge numbers Z. A complete tabulation of values of these susceptibilities for all integer values of Z from the range $1 \leqslant Z \leqslant 137$ has been presented elsewhere [41].

There are two directions in which we would like to extend the current research. First, we plan to analyze various electric and magnetic moments induced in the ground state of the atom by an external, weak, static 2^L-pole *magnetic* field; a result of such an analysis would be a set of static *magnetic* multipole susceptibilities for the atomic ground state. Second, we intend to carry out an analogous study, for both electric and magnetic perturbing fields, for the atom in energetically excited states belonging to the manifold characterized by the principal quantum number $n = 2$. Our preliminary insight into the latter problem shows that such calculations, although significantly more complex than those presented here, should nevertheless be feasible.

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APPENDIX A: MULTIPOLE POLARIZABILITIES VS THE SECOND-ORDER CORRECTION TO THE ATOMIC GROUND-STATE ENERGY

The purpose of this appendix is to give a relationship between the atomic multipole polarizability α_L and the second-order correction to atomic energy due to a perturbing static electric 2^L-pole field defined in Sec. II. It is assumed that before the field was switched on, the atom had been in its ground state.

If we go one step beyond the first-order perturbation theory used in Sec. II, the perturbed wave function of the atom may be approximated by

$$\Psi(\boldsymbol{r}) \simeq \Psi^{(0)}(\boldsymbol{r}) + \Psi^{(1)}(\boldsymbol{r}) + \Psi^{(2)}(\boldsymbol{r}). \tag{A1}$$

The zeroth-order wave function and the first-order correction to it have been given in Eqs. (2.9) and (2.28), respectively; we recall that the first-order perturbation theory has left the coefficients $a_{\pm1/2}$ in Eq. (2.9) undetermined. Similarly, for the atomic energy in the field we may write

$$E \simeq E^{(0)} + E^{(1)} + E^{(2)}, \tag{A2}$$

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

Susceptibility	Related induced moment	Constraints
	Far-field zone	
$\alpha_{\mathrm{E}L\to\mathrm{E}L}$	$\mathsf{Q}_L^{(1)}=(4\pi\epsilon_0)\alpha_{\mathrm{E}L\to\mathrm{E}L}\,\mathsf{C}_L^{(1)}$	
$\alpha_{\mathrm{E}L\to\mathrm{M}\lambda}$	$\mathsf{M}_\lambda^{(1)}=(4\pi\epsilon_0)c\alpha_{\mathrm{E}L\to\mathrm{M}\lambda}\frac{\{\boldsymbol{\nu}\otimes\mathsf{C}_L^{(1)}\}_\lambda}{\langle 10L0\vert\lambda 0\rangle}$	$\lambda=\begin{cases}2 & \text{for } L=1\\ L\mp 1 & \text{for } L\geqslant 2\end{cases}$
$\alpha_{\mathrm{E}L\to\mathrm{T}L}$	$\mathsf{T}_L^{(1)}=i(4\pi\epsilon_0)c\alpha_{\mathrm{E}L\to\mathrm{T}L}\sqrt{L(L+1)}\{\boldsymbol{\nu}\otimes\mathsf{C}_L^{(1)}\}_L$	
	Near-nucleus zone	
$\sigma_{\mathrm{E}L\to\mathrm{E}L}$	$\mathsf{R}_L^{(1)}=(4\pi\epsilon_0)\sigma_{\mathrm{E}L\to\mathrm{E}L}\,\mathsf{C}_L^{(1)}$	
$\sigma_{\mathrm{E}L\to\mathrm{M}\lambda}$	$\mathsf{N}_\lambda^{(1)}=(4\pi\epsilon_0)c\sigma_{\mathrm{E}L\to\mathrm{M}\lambda}\frac{\{\boldsymbol{\nu}\otimes\mathsf{C}_L^{(1)}\}_\lambda}{\langle 10L0\vert\lambda 0\rangle}$	$\lambda=\begin{cases}2 & \text{for } L=1\\ L\mp 1 & \text{for } L\geqslant 2\end{cases}$
$\sigma_{\mathrm{E}L\to\mathrm{T}L}$	$\mathsf{U}_L^{(1)}=i(4\pi\epsilon_0)c\sigma_{\mathrm{E}L\to\mathrm{T}L}\sqrt{L(L+1)}\{\boldsymbol{\nu}\otimes\mathsf{C}_L^{(1)}\}_L$	

with $E^{(0)}$ and $E^{(1)}$ given by Eqs. (2.6) and (2.27), respectively. Proceeding in the standard manner, from Eqs. (2.4), (A1), and (A2) we deduce that the corrections $\Psi^{(2)}(\boldsymbol{r})$ and $E^{(2)}$ solve

$$\left[-ic\hbar\boldsymbol{\alpha}\cdot\boldsymbol{\nabla}+\beta m_e c^2-\frac{Ze^2}{(4\pi\epsilon_0)r}-E^{(0)}\right]\Psi^{(2)}(\boldsymbol{r})=-\left[V_L^{(1)}(\boldsymbol{r})-E^{(1)}\right]\Psi^{(1)}(\boldsymbol{r})+E^{(2)}\Psi^{(0)}(\boldsymbol{r}), \tag{A3}$$

subject to the orthogonality constraints

$$\int_{\mathbb{R}^3}d^3\boldsymbol{r}\;\Psi_m^{(0)\dagger}(\boldsymbol{r})\Psi^{(2)}(\boldsymbol{r})=0\qquad\left(m=\pm\frac{1}{2}\right). \tag{A4}$$

Projecting Eq. (A3) from the left onto the unperturbed basis functions $\Psi_{\pm 1/2}^{(0)}(\boldsymbol{r})$ and then making use of Eqs. (2.9), (2.12), (2.16), (2.27), and (2.28), we arrive at the homogeneous algebraic system

$$\sum_{m'=-1/2}^{1/2}\left[V_{L,mm'}^{(1,1)}-E^{(2)}\delta_{mm'}\right]a_{m'}=0\qquad\left(m=\pm\frac{1}{2}\right), \tag{A5}$$

in which

$$V_{L,mm'}^{(1,1)}=-\int_{\mathbb{R}^3}d^3\boldsymbol{r}\int_{\mathbb{R}^3}d^3\boldsymbol{r}'\;\Psi_m^{(0)\dagger}(\boldsymbol{r})V_L^{(1)}(\boldsymbol{r})\bar{G}^{(0)}(\boldsymbol{r},\boldsymbol{r}')V_L^{(1)}(\boldsymbol{r}')\Psi_{m'}^{(0)}(\boldsymbol{r}'). \tag{A6}$$

To simplify the expression on the right-hand side of Eq. (A6), we make use of Eqs. (2.3), (2.10), (3.13), and (2.20) and also of the definitions (3.16) and (3.15). This yields

$$V_{L,mm'}^{(1,1)}=-(4\pi\epsilon_0)\frac{4\pi}{2L+1}\sum_{\substack{\kappa=-\infty\\(\kappa\neq 0)}}^{\infty}R_\kappa^{(L,L)}(P^{(0)},Q^{(0)};P^{(0)},Q^{(0)})\sum_{M=-L}^{L}\sum_{M'=-L}^{L}\mathcal{C}_{LM}^{(1)*}\mathcal{C}_{LM'}^{(1)*}$$
$$\times\sum_{m_\kappa=-|\kappa|+1/2}^{|\kappa|-1/2}\langle\Omega_{-1m}|Y_{LM}\Omega_{\kappa m_\kappa}\rangle\langle\Omega_{\kappa m_\kappa}|Y_{LM'}\Omega_{-1m'}\rangle. \tag{A7}$$

Evaluation of the angular integrals with the help of Eq. (2.22) casts Eq. (A7) into

$$V_{L,mm'}^{(1,1)}=-(4\pi\epsilon_0)\sum_{\substack{\kappa=-\infty\\(\kappa\neq 0)}}^{\infty}\frac{\delta_{\kappa L}+\delta_{\kappa,-L-1}}{2L+1}R_\kappa^{(L,L)}(P^{(0)},Q^{(0)};P^{(0)},Q^{(0)})\Bigg[\delta_{m,1/2}\delta_{m',1/2}\sum_{M=-L}^{L}(-)^M\frac{\kappa+M}{2\kappa+1}\mathcal{C}_{LM}^{(1)*}\mathcal{C}_{L,-M}^{(1)*}$$
$$-\operatorname{sgn}(\kappa)\delta_{m,1/2}\delta_{m',-1/2}\sum_{M=-L}^{L}(-)^M\frac{\sqrt{(\kappa+M)(\kappa-M+1)}}{|2\kappa+1|}\mathcal{C}_{LM}^{(1)*}\mathcal{C}_{L,-M+1}^{(1)*}-\operatorname{sgn}(\kappa)\delta_{m,-1/2}\delta_{m',1/2}$$
$$\times\sum_{M=-L}^{L}(-)^M\frac{\sqrt{(\kappa-M)(\kappa+M+1)}}{|2\kappa+1|}\mathcal{C}_{LM}^{(1)*}\mathcal{C}_{L,-M-1}^{(1)*}+\delta_{m,-1/2}\delta_{m',-1/2}\sum_{M=-L}^{L}(-)^M\frac{\kappa-M}{2\kappa+1}\mathcal{C}_{LM}^{(1)*}\mathcal{C}_{L,-M}^{(1)*}\Bigg]. \tag{A8}$$

TABLE XVII. 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 ($L \geqslant 1$) electric field $\boldsymbol{\mathcal{E}}_L^{(1)}(\boldsymbol{r})$ derivable from the scalar potential $\varphi_L^{(1)}(\boldsymbol{r})$ defined in Eq. (2.1).

Induced field	Near-zone representation	Far-zone representation
$\phi^{(1)}(\boldsymbol{r})$	$\sigma_{\mathrm{E}L\to\mathrm{E}L}\sqrt{\frac{4\pi}{2L+1}}\, r^{L}\sum_{M=-L}^{L} C_{LM}^{(1)} Y_{LM}^{*}(\boldsymbol{n}_r) = -\sigma_{\mathrm{E}L\to\mathrm{E}L}\varphi_L^{(1)}(\boldsymbol{r})$	$\alpha_{\mathrm{E}L\to\mathrm{E}L}\sqrt{\frac{4\pi}{2L+1}}\, r^{-L-1}\sum_{M=-L}^{L} C_{LM}^{(1)} Y_{LM}^{*}(\boldsymbol{n}_r)$
$\boldsymbol{E}^{(1)}(\boldsymbol{r})$	$-\sigma_{\mathrm{E}L\to\mathrm{E}L}\sqrt{4\pi L}\, r^{L-1}\sum_{M=-L}^{L} C_{LM}^{(1)} \boldsymbol{Y}_{LM}^{L-1*}(\boldsymbol{n}_r) = -\sigma_{\mathrm{E}L\to\mathrm{E}L}\boldsymbol{\mathcal{E}}_L^{(1)}(\boldsymbol{r})$	$-\alpha_{\mathrm{E}L\to\mathrm{E}L}\sqrt{4\pi(L+1)}\, r^{-L-2}\sum_{M=-L}^{L} C_{LM}^{(1)} \boldsymbol{Y}_{LM}^{L+1*}(\boldsymbol{n}_r)$
$\boldsymbol{A}^{(1)}(\boldsymbol{r})$	$-\sum_{\lambda=L\mp1} i c^{-1}\sigma_{\mathrm{E}L\to\mathrm{M}\lambda}(1-\delta_{\lambda0})\sqrt{\frac{4\pi\lambda}{(\lambda+1)(2\lambda+1)}}\, r^{\lambda}\sum_{\mu=-\lambda}^{\lambda}\frac{\{\boldsymbol{\nu}\otimes\mathsf{C}_L^{(1)}\}_{\lambda\mu}}{(10L0\vert\lambda0)}\boldsymbol{Y}_{\lambda\mu}^{\lambda*}(\boldsymbol{n}_r)$	$\sum_{\lambda=L\mp1} i c^{-1}\alpha_{\mathrm{E}L\to\mathrm{M}\lambda}(1-\delta_{\lambda0})\sqrt{\frac{4\pi(\lambda+1)}{\lambda(2\lambda+1)}}\, r^{-\lambda-1}\sum_{\mu=-\lambda}^{\lambda}\frac{\{\boldsymbol{\nu}\otimes\mathsf{C}_L^{(1)}\}_{\lambda\mu}}{(10L0\vert\lambda0)}\boldsymbol{Y}_{\lambda\mu}^{\lambda*}(\boldsymbol{n}_r)$
	$-\, i c^{-1}\sigma_{\mathrm{E}L\to\mathrm{T}L}\sqrt{4\pi(L+1)}\, L r^{L-1}\sum_{M=-L}^{L}\{\boldsymbol{\nu}\otimes\mathsf{C}_L^{(1)}\}_{LM}\boldsymbol{Y}_{LM}^{L-1*}(\boldsymbol{n}_r)$	$-\, i c^{-1}\alpha_{\mathrm{E}L\to\mathrm{T}L}\sqrt{4\pi L}\,(L+1) r^{-L-2}\sum_{M=-L}^{L}\{\boldsymbol{\nu}\otimes\mathsf{C}_L^{(1)}\}_{LM}\boldsymbol{Y}_{LM}^{L+1*}(\boldsymbol{n}_r)$
$\boldsymbol{B}^{(1)}(\boldsymbol{r})$	$-\sum_{\lambda=L\mp1} c^{-1}\sigma_{\mathrm{E}L\to\mathrm{M}\lambda}(1-\delta_{\lambda0})\sqrt{4\pi\lambda}\, r^{\lambda-1}\sum_{\mu=-\lambda}^{\lambda}\frac{\{\boldsymbol{\nu}\otimes\mathsf{C}_L^{(1)}\}_{\lambda\mu}}{(10L0\vert\lambda0)}\boldsymbol{Y}_{\lambda\mu}^{\lambda-1*}(\boldsymbol{n}_r)$	$-\sum_{\lambda=L\mp1} c^{-1}\alpha_{\mathrm{E}L\to\mathrm{M}\lambda}(1-\delta_{\lambda0})\sqrt{4\pi(\lambda+1)}\, r^{-\lambda-2}\sum_{\mu=-\lambda}^{\lambda}\frac{\{\boldsymbol{\nu}\otimes\mathsf{C}_L^{(1)}\}_{\lambda\mu}}{(10L0\vert\lambda0)}\boldsymbol{Y}_{\lambda\mu}^{\lambda+1*}(\boldsymbol{n}_r)$

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

Susceptibility

$$\alpha_{\mathrm{E}L\to\mathrm{E}L} = \frac{a_0^{2L+1}}{Z^{2L+2}} \frac{\Gamma(2\gamma_1+2L+2)}{2^{2L}L(L+1)(2L+1)\Gamma(2\gamma_1+1)} \Bigg\{ 1 + \frac{L^2(L+1)^2(\gamma_1+1)^2\Gamma^2(\gamma_L+\gamma_1+L+1)}{(2L+1)(\gamma_L-\gamma_1+1)\Gamma(2\gamma_1+2L+2)\Gamma(2\gamma_L+1)}\, {}_3F_2\left(\begin{matrix}\gamma_L-\gamma_1-L,\ \gamma_L-\gamma_1-L,\ \gamma_L-\gamma_1+1\\ \gamma_L-\gamma_1+2,\ 2\gamma_L+1\end{matrix};1\right)$$

$$- \frac{(L+1)^2[L(\gamma_1-1)-1]^2\Gamma^2(\gamma_{L+1}+\gamma_1+L+1)}{(2L+1)(\gamma_{L+1}-\gamma_1+1)\Gamma(2\gamma_1+2L+2)\Gamma(2\gamma_{L+1}+1)}\, {}_3F_2\left(\begin{matrix}\gamma_{L+1}-\gamma_1-L,\ \gamma_{L+1}-\gamma_1-L,\ \gamma_{L+1}-\gamma_1+1\\ \gamma_{L+1}-\gamma_1+2,\ 2\gamma_{L+1}+1\end{matrix};1\right)\Bigg\}$$

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

$$\alpha_{\mathrm{E}L\to\mathrm{M}(L+1)} = \frac{\alpha a_0^{2L+2}}{Z^{2L+2}} \frac{(L+1)\Gamma(2\gamma_1+2L+3)}{2^{2L+1}L(2L+1)(2L+3)\Gamma(2\gamma_1+1)} \Bigg\{ 1 + \frac{(L+2)[L(\gamma_1-1)-1]\Gamma(\gamma_{L+1}+\gamma_1+L+1)\Gamma(\gamma_{L+1}+\gamma_1+L+2)}{(\gamma_{L+1}-\gamma_1+1)\Gamma(2\gamma_1+2L+3)\Gamma(2\gamma_{L+1}+1)}$$

$$\times\, {}_3F_2\left(\begin{matrix}\gamma_{L+1}-\gamma_1-L-1,\ \gamma_{L+1}-\gamma_1-L,\ \gamma_{L+1}-\gamma_1+1\\ \gamma_{L+1}-\gamma_1+2,\ 2\gamma_{L+1}+1\end{matrix};1\right)\Bigg\}$$

$$\alpha_{\mathrm{E}L\to\mathrm{T}L} = \frac{\alpha a_0^{2L+2}}{Z^{2L+2}} \frac{1}{2^{2L+1}(2L+1)^2\Gamma(2\gamma_1+1)} \Bigg\{ \frac{(\gamma_1+1)\Gamma(\gamma_L+\gamma_1+L+1)\Gamma(\gamma_L+\gamma_1+L+2)}{(\gamma_L-\gamma_1+1)\Gamma(2\gamma_L+1)}\, {}_3F_2\left(\begin{matrix}\gamma_L-\gamma_1-L-1,\ \gamma_L-\gamma_1-L,\ \gamma_L-\gamma_1+1\\ \gamma_L-\gamma_1+2,\ 2\gamma_L+1\end{matrix};1\right)$$

$$+ \frac{[L(\gamma_1-1)-1]\Gamma(\gamma_{L+1}+\gamma_1+L+1)\Gamma(\gamma_{L+1}+\gamma_1+L+2)}{(L+1)(\gamma_{L+1}-\gamma_1+1)\Gamma(2\gamma_{L+1}+1)}\, {}_3F_2\left(\begin{matrix}\gamma_{L+1}-\gamma_1-L-1,\ \gamma_{L+1}-\gamma_1-L,\ \gamma_{L+1}-\gamma_1+1\\ \gamma_{L+1}-\gamma_1+2,\ 2\gamma_{L+1}+1\end{matrix};1\right)\Bigg\}$$

TABLE XIX. The collection of exact analytical expressions for the near-nucleus static electric multipole susceptibilities for the Dirac one-electron atom in the ground state: the electric nuclear shielding constant $\sigma_{\mathrm{E}L\to\mathrm{E}L}$, the electric-to-magnetic cross susceptibilities $\sigma_{\mathrm{E}L\to\mathrm{M}(L\mp1)}$ and the electric-to-toroidal-magnetic cross susceptibility $\sigma_{\mathrm{E}L\to\mathrm{T}L}$. All the formulas hold for $L \geqslant 1$, except for the one for $\sigma_{\mathrm{E}L\to\mathrm{M}(L-1)}$, which makes physical sense only for $L \geqslant 2$.

Susceptibility	Constraints
$\sigma_{\mathrm{E}L\to\mathrm{E}L} = \frac{2}{ZL(L+1)(2L+1)}\left\{1 + \frac{L^2(L+1)(\gamma_1+1)[\gamma_1(L+1)-L]}{(2L+1)(\gamma_L-\gamma_1+1)(\gamma_L+\gamma_1-L)}\,{}_3F_2\left(\begin{matrix}-L+1, 1, \gamma_L-\gamma_1-L\\ \gamma_L-\gamma_1+2, \gamma_L+\gamma_1-L+1\end{matrix};1\right) - \frac{L(L+1)^2(\gamma_1+1)[L(\gamma_1-1)-1]}{(2L+1)(\gamma_{L+1}-\gamma_1+1)(\gamma_{L+1}+\gamma_1-L)}\,{}_3F_2\left(\begin{matrix}-L+1, 1, \gamma_{L+1}-\gamma_1-L\\ \gamma_{L+1}-\gamma_1+2, \gamma_{L+1}+\gamma_1-L+1\end{matrix};1\right)\right\}$	$Z < \begin{cases}\alpha^{-1} & \text{for } L=1\\ \alpha^{-1}\frac{\sqrt{4L^2-1}}{2L} & \text{for } L \geqslant 2\end{cases}$
$\sigma_{\mathrm{E}L\to\mathrm{M}(L-1)} = -\frac{\alpha a_0}{Z}\frac{L(2\gamma_1+1)}{(L+1)(4L^2-1)}\left\{1 + \frac{(L^2-1)(\gamma_1+1)}{(\gamma_L-\gamma_1+1)(\gamma_L+\gamma_1-L+1)}\,{}_3F_2\left(\begin{matrix}-L+2, 1, \gamma_L-\gamma_1-L\\ \gamma_L-\gamma_1+2, \gamma_L+\gamma_1-L+2\end{matrix};1\right)\right\}$	$L \geqslant 2;\ Z < \alpha^{-1}$
$\sigma_{\mathrm{E}L\to\mathrm{M}(L+1)} = -\frac{\alpha Z}{a_0}\frac{2(L+2)}{\gamma_1 L(2L+1)(2L+3)}\left\{1 - \frac{(L+1)[L(\gamma_1-1)-1]}{(\gamma_{L+1}-\gamma_1+1)(\gamma_{L+1}+\gamma_1-L-1)}\,{}_3F_2\left(\begin{matrix}-L, 1, \gamma_{L+1}-\gamma_1-L\\ \gamma_{L+1}-\gamma_1+2, \gamma_{L+1}+\gamma_1-L\end{matrix};1\right)\right\}$	$Z < \alpha^{-1}\frac{\sqrt{(2L+1)(2L+3)}}{2(L+1)}$
$\sigma_{\mathrm{E}L\to\mathrm{T}L} = -\frac{\alpha a_0}{Z}\frac{(L+1)(2\gamma_1+1)}{L(2L+1)^2}\left\{\frac{\gamma_1+1}{(\gamma_L-\gamma_1+1)(\gamma_L+\gamma_1-L+1)}\,{}_3F_2\left(\begin{matrix}-L+2, 1, \gamma_L-\gamma_1-L\\ \gamma_L-\gamma_1+2, \gamma_L+\gamma_1-L+2\end{matrix};1\right) + \frac{L(\gamma_1-1)-1}{(L+1)(\gamma_{L+1}-\gamma_1+1)(\gamma_{L+1}+\gamma_1-L+1)}\,{}_3F_2\left(\begin{matrix}-L+2, 1, \gamma_{L+1}-\gamma_1-L\\ \gamma_{L+1}-\gamma_1+2, \gamma_{L+1}+\gamma_1-L+2\end{matrix};1\right)\right\}$	$Z < \alpha^{-1}$

The four sums over M may be simplified after evident symmetry properties of their summands are taken into account. One finds that

$$\sum_{M=-L}^{L}(-)^M\frac{\kappa\pm M}{2\kappa+1}\mathcal{C}_{LM}^{(1)*}\mathcal{C}_{L,-M}^{(1)*}=\frac{|\kappa|}{2L+1}\sum_{M=-L}^{L}\mathcal{C}_{LM}^{(1)*}\mathcal{C}_{LM}^{(1)}\quad(\kappa=L,-L-1)\tag{A9}$$

and

$$\sum_{M=-L}^{L}(-)^M\frac{\sqrt{(\kappa\pm M)(\kappa\mp M+1)}}{|2\kappa+1|}\mathcal{C}_{LM}^{(1)*}\mathcal{C}_{L,-M\pm1}^{(1)*}=0\quad(\kappa=L,-L-1).\tag{A10}$$

Hence, we deduce that

$$V_{L,mm'}^{(1,1)}=-\delta_{mm'}(4\pi\epsilon_0)\left[\frac{L}{(2L+1)^2}R_L^{(L,L)}(P^{(0)},Q^{(0)};P^{(0)},Q^{(0)})+\frac{L+1}{(2L+1)^2}R_{-L-1}^{(L,L)}(P^{(0)},Q^{(0)};P^{(0)},Q^{(0)})\right]\sum_{M=-L}^{L}\mathcal{C}_{LM}^{(1)*}\mathcal{C}_{LM}^{(1)}.\tag{A11}$$

The matrix formed by the elements $V_{L,mm'}^{(1,1)}$ is thus seen to be a multiple of the unit 2×2 matrix. Recalling Eqs. (3.24) and (3.25), we are led to the conclusion that application of the second-order perturbation theory does not remove degeneracy of the atomic ground state and that the second-order correction to energy of that state may be written as

$$E^{(2)}=-\tfrac{1}{2}(4\pi\epsilon_0)\alpha_L\mathsf{C}_L^{(1)}\cdot\mathsf{C}_L^{(1)}.\tag{A12}$$

This result is very well known in the dipole ($L=1$) case.

APPENDIX B: FAR-FIELD AND NEAR-FIELD EXPANSIONS OF THE MAGNETIC VECTOR POTENTIAL AND THE MAGNETIC INDUCTION

On our way to a deeper understanding how various sorts of multipole moment tensors arise in the far- and near-field asymptotic expansions of the magnetic vector potential, we have much benefited from studying the methodological paper of Agre [42], which we wholeheartedly recommend to all readers interested in the subject.

1. General considerations

For a given stationary solenoidal current distribution $\boldsymbol{j}(\boldsymbol{r})$, the magnetostatic vector potential may be found from the formula

$$\boldsymbol{A}(\boldsymbol{r})=\frac{\mu_0}{4\pi}\int_{\mathbb{R}^3}d^3\boldsymbol{r}'\,\frac{\boldsymbol{j}(\boldsymbol{r}')}{|\boldsymbol{r}-\boldsymbol{r}'|}.\tag{B1}$$

Exploiting the multipole expansion

$$\frac{1}{|\boldsymbol{r}-\boldsymbol{r}'|}=\sum_{L=0}^{\infty}\sum_{M_L=-L}^{L}\frac{4\pi}{2L+1}\frac{r_<^L}{r_>^{L+1}}Y_{LM_L}^*(\boldsymbol{n}_r)Y_{LM_L}(\boldsymbol{n}_r'),\tag{B2}$$

one finds that in the far-field ($r\to\infty$) and near-field ($r\to0$) regions the vector potential $\boldsymbol{A}(\boldsymbol{r})$ behaves as

$$\boldsymbol{A}(\boldsymbol{r})\xrightarrow{r\to\infty}\sum_{L=0}^{\infty}\boldsymbol{A}^{LL}(\boldsymbol{r})\tag{B3}$$

and

$$\boldsymbol{A}(\boldsymbol{r})\xrightarrow{r\to0}\sum_{L=0}^{\infty}\boldsymbol{A}^{L,-L-1}(\boldsymbol{r}),\tag{B4}$$

respectively, where

$$\boldsymbol{A}^{L\lambda}(\boldsymbol{r})=\frac{\mu_0}{4\pi}\frac{4\pi}{2L+1}r^{-\lambda-1}\sum_{M_L=-L}^{L}Y_{LM_L}^*(\boldsymbol{n}_r)\times\int_{\mathbb{R}^3}d^3\boldsymbol{r}'r'^{\lambda}Y_{LM_L}(\boldsymbol{n}_r')\boldsymbol{j}(\boldsymbol{r}')\quad(\lambda=L,-L-1).\tag{B5}$$

In the next step, we make use of the closure identity

$$\sum_{m=-1}^{1}\boldsymbol{e}_m^*\boldsymbol{e}_m=\mathsf{I}\tag{B6}$$

for the unit vectors of the cyclic basis, which gives

$$\boldsymbol{A}^{L\lambda}(\boldsymbol{r})=\frac{\mu_0}{4\pi}\frac{4\pi}{2L+1}r^{-\lambda-1}\sum_{M_L=-L}^{L}\sum_{m=-1}^{1}Y_{LM_L}^*(\boldsymbol{n}_r)\boldsymbol{e}_m^*\times\int_{\mathbb{R}^3}d^3\boldsymbol{r}'r'^{\lambda}Y_{LM_L}(\boldsymbol{n}_r')\boldsymbol{e}_m\cdot\boldsymbol{j}(\boldsymbol{r}')\quad(\lambda=L,-L-1).\tag{B7}$$

The product $Y_{LM_L}(\boldsymbol{n}_r)\boldsymbol{e}_m$, appearing in Eq. (B7), may be expanded in the basis of vector spherical harmonics as

$$Y_{LM_L}(\boldsymbol{n}_r)\boldsymbol{e}_m=\sum_{J=|L-1|}^{L+1}\sum_{M_J=-J}^{J}\langle LM_L1m|JM_J\rangle\boldsymbol{Y}_{JM_J}^{L}(\boldsymbol{n}_r).\tag{B8}$$

Inserting this relation twice into Eq. (B7) and exploiting the orthonormality property

$$\sum_{M_a=-L_a}^{L_a}\sum_{M_b=-L_b}^{L_b}\langle L_aM_aL_bM_b|JM_J\rangle\langle L_aM_aL_bM_b|J'M_{J'}\rangle=\delta_{JJ'}\delta_{M_JM_{J'}}\tag{B9}$$

of the Clebsch-Gordan coefficients yields

$$\boldsymbol{A}^{L\lambda}(\boldsymbol{r}) = \frac{\mu_0}{4\pi}\frac{4\pi}{2L+1} r^{-\lambda-1} \sum_{J=|L-1|}^{L+1} \sum_{M_J=-J}^{J} \boldsymbol{Y}_{JM_J}^{L*}(\boldsymbol{n}_r) \times \int_{\mathbb{R}^3} d^3\boldsymbol{r}' r'^{\lambda} \boldsymbol{Y}_{JM_J}^{L}(\boldsymbol{n}_r') \cdot \boldsymbol{j}(\boldsymbol{r}') \quad (\lambda = L, -L-1). \tag{B10}$$

If we define

$$\mathcal{Z}_{JM_J}^{L\lambda} = \sqrt{\frac{4\pi}{2L+1}} \int_{\mathbb{R}^3} d^3\boldsymbol{r} r^{\lambda} \boldsymbol{Y}_{JM_J}^{L}(\boldsymbol{n}_r) \cdot \boldsymbol{j}(\boldsymbol{r}) \quad (|L-1| \leqslant J \leqslant L+1), \tag{B11}$$

Eq. (B10) becomes

$$\boldsymbol{A}^{L\lambda}(\boldsymbol{r}) = \frac{\mu_0}{4\pi}\sqrt{\frac{4\pi}{2L+1}} r^{-\lambda-1} \sum_{J=|L-1|}^{L+1} \sum_{M_J=-J}^{J} \mathcal{Z}_{JM_J}^{L\lambda} \boldsymbol{Y}_{JM_J}^{L*}(\boldsymbol{n}_r). \tag{B12}$$

We show that the coefficients $\mathcal{Z}_{JM_J}^{L\lambda}$ are components of a rank-J irreducible spherical tensor $\mathsf{Z}_J^{L\lambda}$. Using the relation

$$\boldsymbol{Y}_{JM_J}^{L}(\boldsymbol{n}_r) = \sum_{M_L=-L}^{L} \sum_{m=-1}^{1} \langle LM_L 1m|JM_J\rangle Y_{LM_L}(\boldsymbol{n}_r)\boldsymbol{e}_m, \tag{B13}$$

reciprocal to the one in Eq. (B8), and the fact that the mth cyclic component of the vector $\boldsymbol{j}(\boldsymbol{r})$ is given by

$$j_m(\boldsymbol{r}) = \boldsymbol{e}_m \cdot \boldsymbol{j}(\boldsymbol{r}), \tag{B14}$$

we obtain

$$\boldsymbol{Y}_{JM_J}^{L}(\boldsymbol{n}_r) \cdot \boldsymbol{j}(\boldsymbol{r}) = \sum_{M_L=-L}^{L} \sum_{m=-1}^{1} \langle LM_L 1m|JM_J\rangle Y_{LM_L}(\boldsymbol{n}_r) j_m(\boldsymbol{r}) = \{\mathsf{Y}_L(\boldsymbol{n}_r) \otimes \boldsymbol{j}(\boldsymbol{r})\}_{JM_J}, \tag{B15}$$

and further

$$\mathcal{Z}_{JM_J}^{L\lambda} = \sqrt{\frac{4\pi}{2L+1}} \int_{\mathbb{R}^3} d^3\boldsymbol{r} r^{\lambda} \{\mathsf{Y}_L(\boldsymbol{n}_r) \otimes \boldsymbol{j}(\boldsymbol{r})\}_{JM_J}, \tag{B16}$$

which proves the statement.

Concluding this section, we observe that since in the definition (B11) J varies in the range $|L-1| \leqslant J \leqslant L+1$, for $L=0$ there are only two tensors in the $\mathsf{Z}_J^{L\lambda}$ family: Z_1^{00} and $\mathsf{Z}_1^{0,-1}$, while for $L \geqslant 1$ their number formally increases to six: Z_{L-1}^{LL}, Z_{L}^{LL}, Z_{L+1}^{LL} and $\mathsf{Z}_{L-1}^{L,-L-1}$, $\mathsf{Z}_{L}^{L,-L-1}$, $\mathsf{Z}_{L+1}^{L,-L-1}$. However, in Secs. B 2 and B 3 of this appendix we show that the tensors Z_{L+1}^{LL} and $\mathsf{Z}_{L-1}^{L,-L-1}$ vanish identically.

2. The far-field case ($\lambda = L$): The tensors M_L and T_{L-1}

In the far-field zone, the asymptotics of the magnetic vector potential is that displayed in Eq. (B3), with $\boldsymbol{A}^{LL}(\boldsymbol{r})$ given by Eq. (B12) specialized to the case $\lambda = L$. Components of the pertinent far-field tensors $\mathsf{Z}_{JM_J}^{LL}$ may be found from Eq. (B11), in which one sets $\lambda = L$.

Consider the tensor $\mathsf{Z}_{L+1,M_{L+1}}^{LL}$. In accordance with what has been said above, its components are given by

$$\mathcal{Z}_{L+1,M_{L+1}}^{LL} = \sqrt{\frac{4\pi}{2L+1}} \int_{\mathbb{R}^3} d^3\boldsymbol{r} r^{L} \boldsymbol{Y}_{L+1,M_{L+1}}^{L}(\boldsymbol{n}_r) \cdot \boldsymbol{j}(\boldsymbol{r}). \tag{B17}$$

However, from the differential relation [40, Eq. (5.8.9)]

$$\nabla[r^{\lambda+1} Y_{JM_J}(\boldsymbol{n}_r)] = (J-\lambda-1)\sqrt{\frac{J+1}{2J+1}} r^{\lambda} \boldsymbol{Y}_{JM_J}^{J+1}(\boldsymbol{n}_r) + (J+\lambda+2)\sqrt{\frac{J}{2J+1}} r^{\lambda} \boldsymbol{Y}_{JM_J}^{J-1}(\boldsymbol{n}_r) \tag{B18}$$

it follows that

$$r^L \boldsymbol{Y}_{L+1,M_{L+1}}^{L}(\boldsymbol{n}_r) = \frac{\nabla[r^{L+1} Y_{L+1,M_{L+1}}(\boldsymbol{n}_r)]}{\sqrt{(L+1)(2L+3)}}. \tag{B19}$$

Consequently, the integrand in Eq. (B17) may be rewritten as

$$r^L \boldsymbol{Y}_{L+1,M_{L+1}}^{L}(\boldsymbol{n}_r) \cdot \boldsymbol{j}(\boldsymbol{r}) = \frac{\nabla \cdot [r^{L+1} Y_{L+1,M_{L+1}}(\boldsymbol{n}_r) \boldsymbol{j}(\boldsymbol{r})]}{\sqrt{(L+1)(2L+3)}} - \frac{r^{L+1} Y_{L+1,M_{L+1}}(\boldsymbol{n}_r) \nabla \cdot \boldsymbol{j}(\boldsymbol{r})}{\sqrt{(L+1)(2L+3)}}. \tag{B20}$$

Since, by assumption, the current is solenoidal, the second term on the right-hand side of Eq. (B20) vanishes. Hence, replacing the integrand in Eq. (B17) with the first term on the right-hand side of Eq. (B20), and then using the Gauss divergence theorem, casts the former equation into

$$\mathcal{Z}_{L+1,M_{L+1}}^{LL} = \sqrt{\frac{4\pi}{(L+1)(2L+1)(2L+3)}} \times \lim_{r\to\infty} \oint_{4\pi} d^2\boldsymbol{n}_r \, r^{L+3} Y_{L+1,M_{L+1}}(\boldsymbol{n}_r) \boldsymbol{n}_r \cdot \boldsymbol{j}(\boldsymbol{r}). \tag{B21}$$

Hence, provided that the current obeys the asymptotic constraint

$$\lim_{r\to\infty} r^{L+3} \boldsymbol{n}_r \cdot \boldsymbol{j}(\boldsymbol{r}) = 0, \tag{B22}$$

one finds that

$$\mathcal{Z}_{L+1,M_{L+1}}^{LL} = 0; \tag{B23}$$

i.e., the tensor Z_{L+1}^{LL} vanishes identically. In result, Eqs. (B3) and (B12) may be combined into

$$\boldsymbol{A}(\boldsymbol{r}) \overset{r\to\infty}{\longrightarrow} \frac{\mu_0}{4\pi} \sum_{L=1}^{\infty} \sqrt{\frac{4\pi}{2L+1}} r^{-L-1} \times \sum_{J=|L-1|}^{L} \sum_{M_J=-J}^{J} \mathcal{Z}_{JM_J}^{LL} \boldsymbol{Y}_{JM_J}^{L*}(\boldsymbol{n}_r) \tag{B24}$$

(the sum starts from $L=1$, as we have proved above that the tensor Z_1^{00} vanishes).

In the literature, instead of the tensors Z_L^{LL} and Z_{L-1}^{LL}, one encounters the tensors M_L and T_{L-1}, components of which, given by

$$\mathcal{M}_{LM_L} = -i\sqrt{\frac{4\pi L}{(L+1)(2L+1)}}\int_{\mathbb{R}^3} d^3\boldsymbol{r}\, r^L \boldsymbol{Y}_{LM_L}^L(\boldsymbol{n}_r)\cdot \boldsymbol{j}(\boldsymbol{r}) \tag{B25}$$

and

$$\mathcal{T}_{L-1,M_{L-1}} = -\frac{1}{2L+1}\sqrt{\frac{4\pi}{L}}\int_{\mathbb{R}^3} d^3\boldsymbol{r}\, r^L \boldsymbol{Y}_{L-1,M_{L-1}}^L(\boldsymbol{n}_r)\cdot \boldsymbol{j}(\boldsymbol{r}), \tag{B26}$$

are related to those of Z_L^{LL} and Z_{L-1}^{LL} through

$$\mathcal{M}_{LM_L} = -i\sqrt{\frac{L}{L+1}}\,\mathcal{Z}_{LM_L}^{LL} \tag{B27}$$

and

$$\mathcal{T}_{L-1,M_{L-1}} = -\frac{1}{\sqrt{L(2L+1)}}\,\mathcal{Z}_{L-1,M_{L-1}}^{LL}. \tag{B28}$$

The tensor M_L is the plain 2^L-pole magnetic moment, and the tensor T_{L-1} is named the 2^{L-1}-pole magnetic toroidal moment [43] (various integral representations of components of the 2^L-pole moment T_L are derived in Appendix C). With the use of components of these two more common tensors, the expansion (B24) is replaced with

$$\begin{aligned}\boldsymbol{A}(\boldsymbol{r}) \stackrel{r\to\infty}{\longrightarrow} \frac{\mu_0}{4\pi}\sum_{L=1}^{\infty}\sqrt{\frac{4\pi}{2L+1}}\,r^{-L-1} &\times\Bigg[i\sqrt{\frac{L+1}{L}}\sum_{M_L=-L}^{L}\mathcal{M}_{LM_L}\boldsymbol{Y}_{LM_L}^{L*}(\boldsymbol{n}_r)\\ &-(1-\delta_{L1})\sqrt{L(2L+1)}\\ &\times\sum_{M_{L-1}=-L+1}^{L-1}\mathcal{T}_{L-1,M_{L-1}}\boldsymbol{Y}_{L-1,M_{L-1}}^{L*}(\boldsymbol{n}_r)\Bigg].\end{aligned} \tag{B29}$$

The factor $1-\delta_{L1}$ has been inserted into the second term in the square bracket since, as shown at the end of Appendix C, it holds that $\mathcal{T}_{00}=0$.

It remains to derive the expression for the asymptotic representation of the magnetic induction with the aid of the well-known formula

$$\boldsymbol{B}(\boldsymbol{r}) = \nabla\times\boldsymbol{A}(\boldsymbol{r}). \tag{B30}$$

If we exploit the differential relation (B18) with $\lambda=-L-1$ and $J=L-1$, this allows us to write the product $r^{-L-1}\boldsymbol{Y}_{L-1,M_{L-1}}^L(\boldsymbol{n}_r)$ as a gradient of a scalar field:

$$r^{-L-1}\boldsymbol{Y}_{L-1,M_{L-1}}^L(\boldsymbol{n}_r) = \frac{\nabla[r^{-L}Y_{L-1,M_{L-1}}(\boldsymbol{n}_r)]}{\sqrt{L(2L-1)}}. \tag{B31}$$

This immediately implies that

$$\nabla\times[r^{-L-1}\boldsymbol{Y}_{L-1,M_{L-1}}^{L*}(\boldsymbol{n}_r)] = \boldsymbol{0}. \tag{B32}$$

On the other hand, from the identity [40, Eq. (7.3.55)]

$$\begin{aligned}\nabla\times[f(r)\boldsymbol{Y}_{LM_L}^L(\boldsymbol{n}_r)] &= i\sqrt{\frac{L}{2L+1}}\left(\frac{\partial}{\partial r}-\frac{L}{r}\right)f(r)\boldsymbol{Y}_{LM_L}^{L+1}(\boldsymbol{n}_r)\\ &+i\sqrt{\frac{L+1}{2L+1}}\left(\frac{\partial}{\partial r}+\frac{L+1}{r}\right)f(r)\boldsymbol{Y}_{LM_L}^{L-1}(\boldsymbol{n}_r)\end{aligned} \tag{B33}$$

one infers that

$$\nabla\times[r^{-L-1}\boldsymbol{Y}_{LM_L}^{L*}(\boldsymbol{n}_r)] = i\sqrt{L(2L+1)}\,r^{-L-2}\boldsymbol{Y}_{LM_L}^{L+1*}(\boldsymbol{n}_r). \tag{B34}$$

On combining Eq. (B30) with Eqs. (B29), (B32), and (B34), one arrives at the sought asymptotic representation

$$\boldsymbol{B}(\boldsymbol{r}) \stackrel{r\to\infty}{\longrightarrow} -\frac{\mu_0}{4\pi}\sum_{L=1}^{\infty}\sqrt{4\pi(L+1)}\,r^{-L-2}\times\sum_{M_L=-L}^{L}\mathcal{M}_{LM_L}\boldsymbol{Y}_{LM_L}^{L+1*}(\boldsymbol{n}_r) \tag{B35}$$

of the magnetic induction. It is seen that components of the magnetic toroidal moments T_L do not appear in Eq. (B35).

3. The near-field case ($\lambda = -L-1$): The tensors N_L and U_{L+1}

In the near-field region, the asymptotic representation of the vector potential may be derived from Eqs. (B4) and (B12), the latter with $\lambda=-L-1$. Components of the tensors $\mathsf{Z}_J^{L,-L-1}$ are given by Eq. (B11), with λ specialized as above. Then, in complete analogy with what has been presented above, the use of the identity (B31) leads to the inference that

$$\mathsf{Z}_{L-1}^{L,-L-1} = 0, \tag{B36}$$

provided that the current is constrained to obey

$$\lim_{r\to 0} r^{-L+2}\boldsymbol{n}_r\cdot\boldsymbol{j}(\boldsymbol{r}) = 0. \tag{B37}$$

If, pursuing further the analogy with the material of Sec. B 2 of this appendix, we introduce the tensors N_L and U_{L+1} with components

$$\mathcal{N}_{LM_L} = i\sqrt{\frac{4\pi(L+1)}{L(2L+1)}}\int_{\mathbb{R}^3} d^3\boldsymbol{r}\, r^{-L-1}\boldsymbol{Y}_{LM_L}^L(\boldsymbol{n}_r)\cdot\boldsymbol{j}(\boldsymbol{r}) \tag{B38}$$

and

$$\mathcal{U}_{L+1,M_{L+1}} = -\frac{1}{2L+1}\sqrt{\frac{4\pi}{L+1}}\times\int_{\mathbb{R}^3} d^3\boldsymbol{r}\, r^{-L-1}\boldsymbol{Y}_{L+1,M_{L+1}}^L(\boldsymbol{n}_r)\cdot\boldsymbol{j}(\boldsymbol{r}), \tag{B39}$$

respectively, related to those of $\mathsf{Z}_L^{L,-L-1}$ and $\mathsf{Z}_{L+1}^{L,-L-1}$ through

$$\mathcal{N}_{LM_L} = i\sqrt{\frac{L+1}{L}}\,\mathcal{Z}_{LM_L}^{L,-L-1} \tag{B40}$$

and

$$\mathcal{U}_{L+1,M_{L+1}} = -\frac{1}{\sqrt{(L+1)(2L+1)}}\,\mathcal{Z}_{L+1,M_{L+1}}^{L,-L-1}, \tag{B41}$$

after some algebra we arrive at the following near-field limit for the vector potential $\boldsymbol{A}(\boldsymbol{r})$:

$$\boldsymbol{A}(\boldsymbol{r}) \xrightarrow{r\to 0} -\frac{\mu_0}{4\pi}\sum_{L=0}^{\infty}\sqrt{\frac{4\pi}{2L+1}}\,r^L \times\Bigg[(1-\delta_{L0})i\sqrt{\frac{L}{L+1}}\sum_{M_L=-L}^{L}\mathcal{N}_{LM_L}\boldsymbol{Y}_{LM_L}^{L*}(\boldsymbol{n}_r) + \sqrt{(L+1)(2L+1)} \times\sum_{M_{L+1}=-L-1}^{L+1}\mathcal{U}_{L+1,M_{L+1}}\boldsymbol{Y}_{L+1,M_{L+1}}^{L*}(\boldsymbol{n}_r)\Bigg]. \tag{B42}$$

The factor $1-\delta_{L0}$ has been inserted into the first term in the square bracket since Eq. (B12) implies that the only nonzero contribution to $\boldsymbol{A}^{0,-1}(\boldsymbol{r})$ comes from the term involving components of the tensor $\mathsf{Z}_1^{0,-1}$ [or equivalently, by virtue of Eq. (B41), the tensor U_1].

The near-field multipole expansion of the magnetic induction is obtained from Eqs. (B30) and (B42), with the aid of the curl identities

$$\nabla\times[r^L\boldsymbol{Y}_{L+1,M_{L+1}}^{L*}(\boldsymbol{n}_r)] = \boldsymbol{0} \tag{B43}$$

[cf. Eq. (B19)] and

$$\nabla\times[r^L\boldsymbol{Y}_{LM_L}^{L*}(\boldsymbol{n}_r)] = -i\sqrt{(L+1)(2L+1)}\,r^{L-1}\boldsymbol{Y}_{LM_L}^{L-1*}(\boldsymbol{n}_r) \tag{B44}$$

[cf. Eq. (B33)]. The required result is

$$\boldsymbol{B}(\boldsymbol{r}) \xrightarrow{r\to 0} -\frac{\mu_0}{4\pi}\sum_{L=1}^{\infty}\sqrt{4\pi L}\,r^{L-1}\sum_{M_L=-L}^{L}\mathcal{N}_{LM_L}\boldsymbol{Y}_{LM_L}^{L-1*}(\boldsymbol{n}_r). \tag{B45}$$

APPENDIX C: ALTERNATIVE INTEGRAL REPRESENTATIONS OF THE FAR-FIELD MAGNETIC TOROIDAL MULTIPOLE MOMENTS T_L

It follows from the material presented in Appendix B that for a given sourceless stationary current distribution $\boldsymbol{j}(\boldsymbol{r})$, spherical components of the magnetic toroidal 2^L-pole moment T_L may be defined as[6]

$$\mathcal{T}_{LM} = -\frac{1}{2L+3}\sqrt{\frac{4\pi}{L+1}}\int_{\mathbb{R}^3} d^3\boldsymbol{r}\,r^{L+1}\boldsymbol{Y}_{LM}^{L+1}(\boldsymbol{n}_r)\cdot\boldsymbol{j}(\boldsymbol{r}), \tag{C1}$$

where $\boldsymbol{Y}_{JM_J}^{L}(\boldsymbol{n}_r)$ denotes the vector spherical harmonic (B13), or equivalently as

$$\mathcal{T}_{LM} = -\frac{1}{2L+3}\sqrt{\frac{4\pi}{L+1}}\int_{\mathbb{R}^3} d^3\boldsymbol{r}\,r^{L+1}\{\mathsf{Y}_{L+1}(\boldsymbol{n}_r)\otimes\boldsymbol{j}(\boldsymbol{r})\}_{LM} \tag{C2}$$

(observe that the irreducible tensor product appearing in the above equation is commutative).

Consider now the identity [40, Eq. (5.8.9)]

$$\nabla[f(r)Y_{LM}(\boldsymbol{n}_r)] = -\sqrt{\frac{L+1}{2L+1}}\left(\frac{\partial}{\partial r}-\frac{L}{r}\right)f(r)\boldsymbol{Y}_{LM}^{L+1}(\boldsymbol{n}_r) + \sqrt{\frac{L}{2L+1}}\left(\frac{\partial}{\partial r}+\frac{L+1}{r}\right)f(r)\boldsymbol{Y}_{LM}^{L-1}(\boldsymbol{n}_r). \tag{C3}$$

In the particular case $f(r)=r^{L+2}$, Eq. (C3) yields

$$\nabla[r^{L+2}Y_{LM}(\boldsymbol{n}_r)] = -2\sqrt{\frac{L+1}{2L+1}}\,r^{L+1}\boldsymbol{Y}_{LM}^{L+1}(\boldsymbol{n}_r) + (2L+3)\sqrt{\frac{L}{2L+1}}\,r^{L+1}\boldsymbol{Y}_{LM}^{L-1}(\boldsymbol{n}_r). \tag{C4}$$

Hence, it follows that Eq. (C1) may be rewritten as

$$\mathcal{T}_{LM} = \frac{\sqrt{\pi(2L+1)}}{(L+1)(2L+3)}\int_{\mathbb{R}^3} d^3\boldsymbol{r}\,\boldsymbol{j}(\boldsymbol{r})\cdot\nabla[r^{L+2}Y_{LM}(\boldsymbol{n}_r)] - \frac{\sqrt{\pi}L}{L+1}\int_{\mathbb{R}^3} d^3\boldsymbol{r}\,r^{L+1}\boldsymbol{Y}_{LM}^{L-1}(\boldsymbol{n}_r)\cdot\boldsymbol{j}(\boldsymbol{r}). \tag{C5}$$

Let us transform the first integrand as follows:

$$\boldsymbol{j}(\boldsymbol{r})\cdot\nabla[r^{L+2}Y_{LM}(\boldsymbol{n}_r)] = \nabla\cdot[r^{L+2}Y_{LM}(\boldsymbol{n}_r)\boldsymbol{j}(\boldsymbol{r})] - r^{L+2}Y_{LM}(\boldsymbol{n}_r)\nabla\cdot\boldsymbol{j}(\boldsymbol{r}). \tag{C6}$$

As we have assumed that the current is sourceless, one has $\nabla\cdot\boldsymbol{j}(\boldsymbol{r})=0$ and the second term on the right-hand side of the above equation is zero. Furthermore, if the current density obeys the constraint

$$\lim_{r\to\infty} r^{L+4}\boldsymbol{n}_r\cdot\boldsymbol{j}(\boldsymbol{r}) = 0 \tag{C7}$$

(which is certainly the case for atomic currents which vanish exponentially at infinity), application of the Gauss' integral theorem to the first term on the right-hand side of Eq. (C6) leads to the inference that the first integral on the right-hand side of Eq. (C5) vanishes. In that way, we have proved that $\mathcal{T}_{LM}$, defined in Eq. (C1) in terms of the vector harmonic $\boldsymbol{Y}_{LM}^{L+1}(\boldsymbol{n}_r)$, may be equivalently expressed as

$$\mathcal{T}_{LM} = -\frac{\sqrt{\pi}L}{L+1}\int_{\mathbb{R}^3} d^3\boldsymbol{r}\,r^{L+1}\boldsymbol{Y}_{LM}^{L-1}(\boldsymbol{n}_r)\cdot\boldsymbol{j}(\boldsymbol{r}). \tag{C8}$$

Multiplying Eq. (C8) by $\eta\in\mathbb{C}$ and Eq. (C1) by $1-\eta$, and then adding, we find

$$\mathcal{T}_{LM} = -\sqrt{\frac{\pi}{L+1}}\int_{\mathbb{R}^3} d^3\boldsymbol{r}\,r^{L+1}\Bigg[\eta\sqrt{\frac{L}{L+1}}\boldsymbol{Y}_{LM}^{L-1}(\boldsymbol{n}_r) + (1-\eta)\frac{2}{2L+3}\boldsymbol{Y}_{LM}^{L+1}(\boldsymbol{n}_r)\Bigg]\cdot\boldsymbol{j}(\boldsymbol{r}). \tag{C9}$$

Playing with the value of η, the above general formula may be used to obtain particular expressions for $\mathcal{T}_{LM}$, some of which have already appeared in the literature. For instance,

[6] The components of the magnetic toroidal multipole moments defined in Refs. [42,43] are complex conjugates of ours. Moreover, in Refs. [42,43] the Gauss system of units was used, while in this paper we conform to the International System of Units; consequently, we omit the factor $1/c$ in the definition of $\mathcal{T}_{LM}$.

with $\eta = (L+1)/(2L+1)$ Eq. (C9) becomes

$$\mathcal{T}_{LM} = -\frac{\sqrt{\pi}L}{2L+1}\int_{\mathbb{R}^3} d^3\boldsymbol{r}\, r^{L+1} \times \left[\boldsymbol{Y}_{LM}^{L-1}(\boldsymbol{n}_r) + \frac{2}{2L+3}\sqrt{\frac{L}{L+1}}\boldsymbol{Y}_{LM}^{L+1}(\boldsymbol{n}_r)\right]\cdot \boldsymbol{j}(\boldsymbol{r}), \tag{C10}$$

which coincides with Eq. (4.10) in Ref. [43]. Furthermore, if $\eta = -2/(2L+1)$, then Eq. (C9) reduces to

$$\mathcal{T}_{LM} = \frac{1}{L+1}\sqrt{\frac{4\pi}{2L+1}}\int_{\mathbb{R}^3} d^3\boldsymbol{r}\, r^{L+1} \times \left[\sqrt{\frac{L}{2L+1}}\boldsymbol{Y}_{LM}^{L-1}(\boldsymbol{n}_r) - \sqrt{\frac{L+1}{2L+1}}\boldsymbol{Y}_{LM}^{L+1}(\boldsymbol{n}_r)\right]\cdot \boldsymbol{j}(\boldsymbol{r}). \tag{C11}$$

Since it is known (cf. Ref. [40, Eq. (7.3.70)]) that

$$\sqrt{\frac{L}{2L+1}}\boldsymbol{Y}_{LM}^{L-1}(\boldsymbol{n}_r) - \sqrt{\frac{L+1}{2L+1}}\boldsymbol{Y}_{LM}^{L+1}(\boldsymbol{n}_r) = \boldsymbol{n}_r Y_{LM}(\boldsymbol{n}_r), \tag{C12}$$

Eq. (C11) may be rewritten in the compact form

$$\mathcal{T}_{LM} = \frac{1}{L+1}\sqrt{\frac{4\pi}{2L+1}}\int_{\mathbb{R}^3} d^3\boldsymbol{r}\, r^{L} Y_{LM}(\boldsymbol{n}_r)\boldsymbol{r}\cdot \boldsymbol{j}(\boldsymbol{r}), \tag{C13}$$

given before in Refs. [43, Eq. (B.4)] and [25, Eq. (2.2)]. The representation (C13) of $\mathcal{T}_{LM}$ has been found to be most suitable for the purposes of this work, and the considerations presented in Sec. V have been based upon it. As the last example, in Eq. (C9) we put $\eta = 2(L+1)/[(L+2)(2L+1)]$. This casts the latter equation into

$$\mathcal{T}_{LM} = -\frac{1}{L+2}\sqrt{\frac{4\pi L}{(L+1)(2L+1)}}\int_{\mathbb{R}^3} d^3\boldsymbol{r}\, r^{L+1} \times \left[\sqrt{\frac{L+1}{2L+1}}\boldsymbol{Y}_{LM}^{L-1}(\boldsymbol{n}_r) + \sqrt{\frac{L}{2L+1}}\boldsymbol{Y}_{LM}^{L+1}(\boldsymbol{n}_r)\right]\cdot \boldsymbol{j}(\boldsymbol{r}). \tag{C14}$$

The integrand in Eq. (C14) may be simplified with the aid of the formula (cf. Ref. [40, Eq. (7.3.73)])

$$\sqrt{\frac{L+1}{2L+1}}\boldsymbol{Y}_{LM}^{L-1}(\boldsymbol{n}_r) + \sqrt{\frac{L}{2L+1}}\boldsymbol{Y}_{LM}^{L+1}(\boldsymbol{n}_r) = -i\boldsymbol{n}_r \times \boldsymbol{Y}_{LM}^{L}(\boldsymbol{n}_r). \tag{C15}$$

This yields

$$\mathcal{T}_{LM} = -\frac{i}{L+2}\sqrt{\frac{4\pi L}{(L+1)(2L+1)}} \times \int_{\mathbb{R}^3} d^3\boldsymbol{r}\, r^{L}\boldsymbol{Y}_{LM}^{L}(\boldsymbol{n}_r)\cdot[\boldsymbol{r}\times \boldsymbol{j}(\boldsymbol{r})]. \tag{C16}$$

Since it holds that [40, Eqs. (7.3.9) and (7.3.6)]

$$\boldsymbol{Y}_{LM}^{L}(\boldsymbol{n}_r) = \frac{\boldsymbol{\Lambda}Y_{LM}(\boldsymbol{n}_r)}{\sqrt{L(L+1)}}, \tag{C17}$$

the third particular expression for $\mathcal{T}_{LM}$ we wish to present here is

$$\mathcal{T}_{LM} = \frac{i}{(L+1)(L+2)}\sqrt{\frac{4\pi}{2L+1}} \times \int_{\mathbb{R}^3} d^3\boldsymbol{r}\, r^{L} Y_{LM}(\boldsymbol{n}_r)\boldsymbol{\Lambda}\cdot[\boldsymbol{r}\times \boldsymbol{j}(\boldsymbol{r})]. \tag{C18}$$

Concluding this appendix, we observe that the monopole toroidal moment vanishes identically. This is immediately seen if in Eq. (C13) one sets $L = M = 0$, obtaining

$$\mathcal{T}_{00} = \int_{\mathbb{R}^3} d^3\boldsymbol{r}\, \boldsymbol{r}\cdot \boldsymbol{j}(\boldsymbol{r}), \tag{C19}$$

and then one replaces the integrand by the right-hand side of the obvious identity

$$\boldsymbol{r}\cdot \boldsymbol{j}(\boldsymbol{r}) = \frac{1}{2}\nabla\cdot[r^2\boldsymbol{j}(\boldsymbol{r})] - \frac{1}{2}r^2\nabla\cdot \boldsymbol{j}(\boldsymbol{r}). \tag{C20}$$

APPENDIX D: ALTERNATIVE INTEGRAL REPRESENTATIONS OF THE NEAR-FIELD MAGNETIC TOROIDAL MULTIPOLE MOMENTS U_L

In Appendix B, we have come across a set of the near-nucleus magnetic toroidal multipole moments U_L, with $L \geqslant 1$, the spherical components of which are given by

$$\mathcal{U}_{LM} = -\frac{1}{2L-1}\sqrt{\frac{4\pi}{L}}\int_{\mathbb{R}^3} d^3\boldsymbol{r}\, r^{-L}\boldsymbol{Y}_{LM}^{L-1}(\boldsymbol{n}_r)\cdot \boldsymbol{j}(\boldsymbol{r}), \tag{D1}$$

or equivalently by

$$\mathcal{U}_{LM} = -\frac{1}{2L-1}\sqrt{\frac{4\pi}{L}}\int_{\mathbb{R}^3} d^3\boldsymbol{r}\, r^{-L}\{\mathsf{Y}_{L-1}(\boldsymbol{n}_r)\otimes \boldsymbol{j}(\boldsymbol{r})\}_{LM}. \tag{D2}$$

In this appendix, we aim to show that there is a one-parameter family of representations of $\mathcal{U}_{LM}$ which, under some constraints imposed on the current density $\boldsymbol{j}(\boldsymbol{r})$, are equivalent to the one given in Eq. (D1). We shall be brief, as in many details the reasoning is similar to that presented in Appendix C, where the counterpart set of the far-field moments has been considered.

Substitution of $f(r) = r^{-L+1}$ into Eq. (C3) transforms the latter into

$$\nabla[r^{-L+1}Y_{LM}(\boldsymbol{n}_r)] = (2L-1)\sqrt{\frac{L+1}{2L+1}}r^{-L}\boldsymbol{Y}_{LM}^{L+1}(\boldsymbol{n}_r) + 2\sqrt{\frac{L}{2L+1}}r^{-L}\boldsymbol{Y}_{LM}^{L-1}(\boldsymbol{n}_r); \tag{D3}$$

hence, it follows that Eq. (D1) may be rewritten as

$$\mathcal{U}_{LM} = -\frac{\sqrt{\pi(2L+1)}}{L(2L-1)}\int_{\mathbb{R}^3} d^3\boldsymbol{r}\, \boldsymbol{j}(\boldsymbol{r})\cdot\nabla[r^{-L+1}Y_{LM}(\boldsymbol{n}_r)] + \frac{\sqrt{\pi(L+1)}}{L}\int_{\mathbb{R}^3} d^3\boldsymbol{r}\, r^{-L}\boldsymbol{Y}_{LM}^{L+1}(\boldsymbol{n}_r)\cdot \boldsymbol{j}(\boldsymbol{r}). \tag{D4}$$

Now it is evident that

$$\boldsymbol{j}(\boldsymbol{r})\cdot\nabla[r^{-L+1}Y_{LM}(\boldsymbol{n}_r)] = \nabla\cdot[r^{-L+1}Y_{LM}(\boldsymbol{n}_r)\boldsymbol{j}(\boldsymbol{r})] - r^{-L+1}Y_{LM}(\boldsymbol{n}_r)\nabla\cdot \boldsymbol{j}(\boldsymbol{r}). \tag{D5}$$

Consequently, if the current is solenoidal and such that

$$\lim_{r\to 0} r^{-L+3}\boldsymbol{n}_r \cdot \boldsymbol{j}(\boldsymbol{r}) = 0, \quad \lim_{r\to\infty} r^{-L+3}\boldsymbol{n}_r \cdot \boldsymbol{j}(\boldsymbol{r}) = 0, \tag{D6}$$

the first integral on the right-hand side of Eq. (D4) vanishes, yielding

$$\mathcal{U}_{LM} = \frac{\sqrt{\pi(L+1)}}{L}\int_{\mathbb{R}^3} d^3\boldsymbol{r}\, r^{-L}\boldsymbol{Y}_{LM}^{L+1}(\boldsymbol{n}_r)\cdot \boldsymbol{j}(\boldsymbol{r}). \tag{D7}$$

Multiplying Eq. (D1) by a parameter $\eta \in \mathbb{C}$ and Eq. (D7) by $1-\eta$, and then adding, we obtain the sought one-parameter family of equivalent expressions

$$\mathcal{U}_{LM} = -\sqrt{\frac{\pi}{L}}\int_{\mathbb{R}^3} d^3\boldsymbol{r}\, r^{-L}\left[\eta\frac{2}{2L-1}\boldsymbol{Y}_{LM}^{L-1}(\boldsymbol{n}_r) - (1-\eta)\sqrt{\frac{L+1}{L}}\boldsymbol{Y}_{LM}^{L+1}(\boldsymbol{n}_r)\right]\cdot \boldsymbol{j}(\boldsymbol{r}), \tag{D8}$$

which may be interchangeably used as definitions of components of the tensor U_L.

Two particular choices of η are worth analyzing here. Thus, for

$$\eta = \frac{2L-1}{2L+1}, \tag{D9}$$

by virtue of the identity (C12), we obtain

$$\mathcal{U}_{LM} = -\frac{1}{L}\sqrt{\frac{4\pi}{2L+1}}\int_{\mathbb{R}^3} d^3\boldsymbol{r}\, r^{-L-1}Y_{LM}(\boldsymbol{n}_r)\boldsymbol{r}\cdot \boldsymbol{j}(\boldsymbol{r}), \tag{D10}$$

while for

$$\eta = \frac{(L+1)(2L-1)}{(L-1)(2L+1)} \quad (L \neq 1), \tag{D11}$$

after exploiting the relations (C15) and (C17), we find

$$\mathcal{U}_{LM} = \frac{i}{L(L-1)}\sqrt{\frac{4\pi}{2L+1}}\int_{\mathbb{R}^3} d^3\boldsymbol{r}\, r^{-L-1}Y_{LM}(\boldsymbol{n}_r)\boldsymbol{\Lambda}\cdot[\boldsymbol{r}\times \boldsymbol{j}(\boldsymbol{r})] \quad (L\neq 1). \tag{D12}$$

If $L=1$ were admitted in Eq. (D12), the integral appearing therein would vanish (see the next paragraph), and consequently on the right-hand side we would have a 0/0-type expression. To prepare the ground for the use of the L'Hospital rule, we set $L=1$ in the spherical harmonic and $L=1+\varepsilon$ at other places in the above formula. Hence, if we let ε tend to zero, after exploiting the aforementioned rule, we obtain

$$\mathcal{U}_{1M} = -i\sqrt{\frac{4\pi}{3}}\int_{\mathbb{R}^3} d^3\boldsymbol{r}\, r^{-2}\ln(r/r_0)Y_{1M}(\boldsymbol{n}_r)\boldsymbol{\Lambda}\cdot[\boldsymbol{r}\times \boldsymbol{j}(\boldsymbol{r})], \tag{D13}$$

where r_0, of the dimension of length and such that $r_0 > 0$ but otherwise arbitrary, has been introduced merely to make the argument of the logarithm physically dimensionless.

We still owe the reader a proof that $I_{1M}=0$, where

$$I_{1M} = \int_{\mathbb{R}^3} d^3\boldsymbol{r}\, r^{-2}Y_{1M}(\boldsymbol{n}_r)\boldsymbol{\Lambda}\cdot[\boldsymbol{r}\times \boldsymbol{j}(\boldsymbol{r})]. \tag{D14}$$

To show this, we observe that with the use of the relation

$$Y_{1M}(\boldsymbol{n}_r) = \sqrt{\frac{3}{4\pi}}\,\boldsymbol{e}_M\cdot\boldsymbol{n}_r \tag{D15}$$

the integral in Eq. (D14) may be transformed into

$$I_{1M} = \sqrt{\frac{3}{4\pi}}\int_{\mathbb{R}^3} d^3\boldsymbol{r}\, r^{-3}[(\boldsymbol{r}\times\boldsymbol{\Lambda})(\boldsymbol{e}_M\cdot\boldsymbol{r})]\cdot \boldsymbol{j}(\boldsymbol{r}). \tag{D16}$$

Hence, it follows that

$$I_{1M} = -i\sqrt{\frac{3}{4\pi}}\int_{\mathbb{R}^3} d^3\boldsymbol{r}\,\frac{\boldsymbol{n}_r\times(\boldsymbol{n}_r\times\boldsymbol{e}_M)}{r}\cdot \boldsymbol{j}(\boldsymbol{r}). \tag{D17}$$

Now, it holds that

$$\frac{\boldsymbol{n}_r\times(\boldsymbol{n}_r\times\boldsymbol{e}_M)}{r} = -\boldsymbol{\nabla}(\boldsymbol{e}_M\cdot\boldsymbol{n}_r), \tag{D18}$$

and consequently one has

$$I_{1M} = i\sqrt{\frac{3}{4\pi}}\int_{\mathbb{R}^3} d^3\boldsymbol{r}\,\boldsymbol{\nabla}\cdot[(\boldsymbol{e}_M\cdot\boldsymbol{n}_r)\boldsymbol{j}(\boldsymbol{r})] - i\sqrt{\frac{3}{4\pi}}\int_{\mathbb{R}^3} d^3\boldsymbol{r}(\boldsymbol{e}_M\cdot\boldsymbol{n}_r)\boldsymbol{\nabla}\cdot \boldsymbol{j}(\boldsymbol{r}). \tag{D19}$$

The first integral on the right-hand side is zero by virtue of the Gauss' theorem and the constraints in Eq. (D6), while in the second one the integrand vanishes identically since, by assumption, the current is sourceless. This completes the proof.

APPENDIX E: FORMULAS FOR THE GENERALIZED HYPERGEOMETRIC SERIES ${}_3F_2(a,1,1;b,n;1)$ WITH $n=3,4,5$

In the course of evaluation of the three kinds of shielding factors, presented in Secs. VI to VIII, we have encountered the specialized generalized hypergeometric series ${}_3F_2(a,1,1;b,n;1)$, with $n=3,4,5$. It may be found in the literature that the one with $n=3$ may be expressed in terms of the digamma function as [44, Eq. (7.4.4.41)]

$${}_3F_2\left(\begin{matrix}a,1,1\\b,3\end{matrix};1\right) = \frac{2(b-1)}{a-1} - \frac{2(b-1)(b-a)}{(a-1)(a-2)}[\psi(b-1)-\psi(b-a+1)] \quad [\mathrm{Re}(b-a) > -1], \tag{E1}$$

which, after exploiting the relation

$$\psi(z+1) = \psi(z) + \frac{1}{z}, \tag{E2}$$

may be transformed into

$${}_3F_2\left(\begin{matrix}a,1,1\\b,3\end{matrix};1\right) = \frac{2(b-1)}{a-2} - \frac{2(b-1)(b-a)}{(a-1)(a-2)}[\psi(b-1)-\psi(b-a)] \quad [\mathrm{Re}(b-a) > -1]. \tag{E3}$$

Below we derive analogous expressions for the two remaining ${}_3F_2(1)$ functions of interest in the context of this work.

Playing with the definition

$$ {}_3F_2\left(\begin{matrix} a_1, a_2, a_3 \\ b_1, b_2 \end{matrix}; z\right) = \frac{\Gamma(b_1)\Gamma(b_2)}{\Gamma(a_1)\Gamma(a_2)\Gamma(a_3)} \sum_{n=0}^{\infty} \frac{\Gamma(n+a_1)\Gamma(n+a_2)\Gamma(n+a_3)}{\Gamma(n+b_1)\Gamma(n+b_2)} \frac{z^n}{n!} $$

$$ [|z| \leqslant 1;\ \mathrm{Re}(b_1+b_2-a_1-a_2-a_3) > 0 \text{ for } z=1] \tag{E4} $$

(the constraints on z, a's and b's are tacitly assumed to hold throughout the rest of this appendix), it is possible to obtain the recurrence relation

$$ {}_3F_2\left(\begin{matrix} a_1, a_2, a_3 \\ b_1, b_2 \end{matrix}; z\right) = \frac{a_3}{a_3-b_2+1}\, {}_3F_2\left(\begin{matrix} a_1, a_2, a_3+1 \\ b_1, b_2 \end{matrix}; z\right) - \frac{b_2-1}{a_3-b_2+1}\, {}_3F_2\left(\begin{matrix} a_1, a_2, a_3 \\ b_1, b_2-1 \end{matrix}; z\right), \tag{E5} $$

from which we deduce that

$$ {}_3F_2\left(\begin{matrix} a, 1, 1 \\ b, n \end{matrix}; 1\right) = -\frac{1}{n-2}\, {}_3F_2\left(\begin{matrix} a, 1, 2 \\ b, n \end{matrix}; 1\right) + \frac{n-1}{n-2}\, {}_3F_2\left(\begin{matrix} a, 1, 1 \\ b, n-1 \end{matrix}; 1\right). \tag{E6} $$

Next we exploit the identity

$$ {}_3F_2\left(\begin{matrix} a_1, 1, a_3 \\ b_1, b_2 \end{matrix}; z\right) = \frac{(b_1-1)(b_2-1)}{(a_1-1)(a_3-1)z}\, {}_3F_2\left(\begin{matrix} a_1-1, 1, a_3-1 \\ b_1-1, b_2-1 \end{matrix}; z\right) - \frac{(b_1-1)(b_2-1)}{(a_1-1)(a_3-1)z}, \tag{E7} $$

which also may be directly inferred from the definition (E4). As the particular case of that identity, we have

$$ {}_3F_2\left(\begin{matrix} a, 1, 2 \\ b, n \end{matrix}; 1\right) = \frac{(n-1)(b-1)}{a-1}\, {}_3F_2\left(\begin{matrix} a-1, 1, 1 \\ b-1, n-1 \end{matrix}; 1\right) - \frac{(n-1)(b-1)}{a-1}. \tag{E8} $$

Insertion of Eq. (E8) into Eq. (E6) yields the relationship

$$ {}_3F_2\left(\begin{matrix} a, 1, 1 \\ b, n \end{matrix}; 1\right) = \frac{n-1}{n-2}\, {}_3F_2\left(\begin{matrix} a, 1, 1 \\ b, n-1 \end{matrix}; 1\right) - \frac{(n-1)(b-1)}{(n-2)(a-1)}\, {}_3F_2\left(\begin{matrix} a-1, 1, 1 \\ b-1, n-1 \end{matrix}; 1\right) + \frac{(n-1)(b-1)}{(n-2)(a-1)}. \tag{E9} $$

If in Eq. (E9) we put $n=4$, after simplifying the right-hand side with the use of Eqs. (E3) and (E2), we obtain

$$ {}_3F_2\left(\begin{matrix} a, 1, 1 \\ b, 4 \end{matrix}; 1\right) = \frac{3(b-1)(3a-2b-4)}{2(a-2)(a-3)} + \frac{3(b-1)(b-a)(b-a+1)}{(a-1)(a-2)(a-3)}[\psi(b-1)-\psi(b-a)] \quad [\mathrm{Re}(b-a) > -2]. \tag{E10} $$

Employing Eq. (E9) recursively, in the similar manner we find

$$ {}_3F_2\left(\begin{matrix} a, 1, 1 \\ b, 5 \end{matrix}; 1\right) = \frac{2(b-1)(6b^2+24b-15ab-40a+11a^2+36)}{3(a-2)(a-3)(a-4)} - \frac{4(b-1)(b-a)(b-a+1)(b-a+2)}{(a-1)(a-2)(a-3)(a-4)}[\psi(b-1)-\psi(b-a)] \quad [\mathrm{Re}(b-a) > -3]. \tag{E11} $$

For the sake of completeness, we observe that apparent singularities at some values of the parameter a in the expressions on the right-hand sides of Eqs. (E3), (E10), and (E11) are removable with an application of the L'Hospital rule.

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