Static electric multipole susceptibilities of the relativistic hydrogen-like atom in the ground state: Application of the Sturmian expansion of the generalized Dirac–Coulomb Green function

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Abstract

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 30 (1997) 825, erratum: 30 (1997) 2747] 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 $\alpha_L$, electric-to-magnetic cross-susceptibilities $\alpha_{E \rightarrow M}(L \pm 1)$ and electric-to-toroidal-magnetic cross-susceptibilities $\alpha_{E \rightarrow T L}$ — are found to be expressible in terms of one or two non-terminating generalized hypergeometric functions $3F_2$ with the unit argument. Counterpart formulas for the near-nucleus multipole susceptibilities — the electric nuclear shielding constants $\sigma_{E \rightarrow E}(L \pm 1)$, near-nucleus electric-to-magnetic cross-susceptibilities $\sigma_{E \rightarrow M}(L \pm 1)$ and near-nucleus electric-to-toroidal-magnetic cross-susceptibilities $\sigma_{E \rightarrow T L}$ — involve terminating $3F_2(1)$ series and for each $L$ may be rewritten in terms of elementary functions. Exact numerical values of the far-field dipole, quadrupole, octupole and hexadecapole susceptibilities are provided for selected hydrogenic ions. Analytical quasi-relativistic approximations, valid to the second order in $\alpha Z$, where $\alpha$ is the fine-structure constant and $Z$ is the nuclear charge number, are derived for all types of the far-field and near-nucleus susceptibilities considered in the paper.

Key words: polarizabilities; nuclear shielding constants; cross-susceptibilities; electromagnetic susceptibilities; multipole moments; toroidal moments; Dirac one-electron atom; Dirac–Coulomb Green function; Sturmian functions

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1 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 early 1970s, when Zon et al. [1] presented a closed-form analytical expression for the dipole polarizability $\alpha_1$ 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 $\alpha_1$ were derived, with the use of various alternative analytical techniques, by Labzowsky [2,3], Shestakov

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and Khristenko [4], Labzowsky et al. [5], Le Anh Thu et al. [6], Szymtkowski [7], Yakhontov [8], and Szymtkowski and Mielewczyk [9]. Quasi-relativistic approximations to \( \alpha_L \), correct to the second order in \( \alpha Z \), where \( \alpha \) 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 \( \alpha_L \); the formula involved altogether eight different \( 3P_L(1) \) 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 quasi-relativistic representation for \( \alpha_L \), given by Kaneko in Ref. [17] and by Drachman in an erratum to Ref. [18], coincided with the corresponding limit deduced in Ref. [14].

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 \( \alpha_1 \), employing the Slater-type functions used as a variational basis set. Zhang et al. [20] presented results for the quadrupole polarizability \( \alpha_2 \) computed with the use of the B-spline Galerkin method. The latter study was pushed further in Ref. [21], where numerical data for \( \alpha_L \) with \( 1 \leq L \leq 4 \) were provided. Finally, very recently Filippin et al. [22] applied their Lagrange-mesh method in computations of \( \alpha_L \), 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 \( \alpha_L \) 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 electric-to-toroidal-magnetic multipole cross-susceptibilities. In Ref. [23], Szymtkowski and Stefanińska derived an exact closed-form analytical expression for the electric-dipole-to-magnetic-quadrupole cross-susceptibility \( \sigma_{E1\rightarrow M2} \) 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 \( \sigma_{E1\rightarrow T1} \) may be inferred from the papers of Lewis and Blinder [24] and Mielewczyk and Szymtkowski [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 \( \sigma_{EL\rightarrow EL} \). 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 quasi-relativistic estimates for the shielding constants with \( L = 2 \) and \( L = 3 \) were deduced [16][26]. Moreover, a quasi-relativistic formula for \( \sigma_{EL\rightarrow EL} \) 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

\[ \text{References} \]

1 It should be mentioned that a quasi-relativistic expression for \( \alpha_2 \) given in Ref. [12] is incorrect and that the criticism of the work [17] presented in an appendix to Ref. [12] was mostly unjustified.
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 \(\alpha_L\) and \(\sigma_{EL \rightarrow EL}\), 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 2 provides some basic notions and facts concerning the ground state of the Dirac one-electron atom placed in a \(2L\)-pole electric field. In Secs. 3–5, 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 (quasi-relativistic) expressions for the multipole susceptibilities (the polarizabilities, the electric-to-magnetic cross-susceptibilities) and also tabulate their numerical values computed from the exact formulas for selected values of the nuclear charge \(Z\). Analogous considerations concerning the near-field moments and the susceptibilities related to them are carried out in Secs. 6–8. The final Sec. 9 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 appendices. 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 Appendices B and C 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 they emerge in. Some properties of the generalized hypergeometric function \(3F_2\) with the unit argument, relevant to the material presented in Secs. 6–8 are discussed in Appendix E.

## 2 Preliminaries

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

\[
\varphi_L^{(1)}(\mathbf{r}) = -\sqrt{\frac{4\pi}{2L + 1}} r^L C_L^{(1)} \cdot \mathbf{Y}_L(n_r) \quad (L \geq 1),
\]

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

\[
C_{LM}^{(1)} = (-)^M c_L^{(1)} c_{L,-M},
\]

where the asterisk denotes the complex conjugation.\(^2\) This ensures that \(\varphi_L^{(1)}(\mathbf{r})\) is real. In terms of components of the two tensors, the interaction energy between the atomic electron and the field

\[\text{energy} = -\int d^3r \mathbf{r} \cdot \mathbf{E}^{(1)}(\mathbf{r}),\]

is given by the contribution of the atom in a \(2L\)-pole field
reads
\[ V_L^{(1)}(r) = e \sqrt{\frac{4\pi}{2L + 1}} \sum_{M=-L}^{L} c_{LM}^{(1)} Y_{LM}(n_r) \quad (L \geq 1). \tag{2.3} \]

Henceforth, it will be assumed that the electric force \(-\nabla V_L^{(1)}(r)\) 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
\[ \left[ -i\hbar \alpha \cdot \nabla + \beta mc^2 - \frac{Ze^2}{4\pi \epsilon_0} r + V_L^{(1)}(r) - E \right] \Psi(r) = 0, \tag{2.4} \]
where \(\alpha\) and \(\beta\) 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 \(V_L^{(1)}(r)\) will be considered as a small perturbation of the Dirac–Coulomb Hamiltonian. Then, to the first order in that perturbation, the energy eigenvalue is
\[ E \approx E^{(0)} + E^{(1)}, \tag{2.5} \]
with the (doubly-degenerate) unperturbed ground-state energy level \(E^{(0)}\) given by
\[ E^{(0)} = mc^2 \gamma_1, \tag{2.6} \]
where
\[ \gamma_\alpha = \sqrt{\kappa^2 - (\alpha Z)^2} \tag{2.7} \]
\((\alpha, \text{not to be confused with the Dirac matrix } \alpha \text{ or the multipole polarizability } \alpha_L, \text{is the Sommerfeld fine-structure constant}). To the same order, the electron wave function is
\[ \Psi(r) \approx \Psi^{(0)}(r) + \Psi^{(1)}(r), \tag{2.8} \]
with the unperturbed component given by
\[ \Psi^{(0)}(r) = a_{1/2} \Psi^{(0)}_{1/2}(r) + a_{-1/2} \Psi^{(0)}_{-1/2}(r). \tag{2.9} \]

The basis states \(\Psi^{(0)}_m(r)\) appearing in Eq. (2.9) are chosen to be
\[ \Psi^{(0)}_m(r) = \frac{1}{r} \left( \begin{array}{c} P^{(0)}(r) \Omega_{-1m}(n_r) \\ iQ^{(0)}(r) \Omega_{1m}(n_r) \end{array} \right) \tag{2.10} \]
where
\[ P^{(0)}(r) = -\frac{Z}{a_0} \left( 1 + \frac{1}{\gamma_1} \right) \frac{2Zr}{a_0} \gamma_1 e^{-Zr/a_0}, \tag{2.11a} \]
\[ Q^{(0)}(r) = \frac{Z}{a_0} \left( 1 - \frac{1}{\gamma_1} \right) \frac{2Zr}{a_0} \gamma_1 e^{-Zr/a_0}, \tag{2.11b} \]
while \(\Omega_{\kappa m_n}(n_r)\) are the spherical spinors \[35\]. It is easy to verify that the functions (2.10) are orthonormal in the sense of
\[ \int_{\mathbb{R}^3} d^3r \, \Psi^{(0)}_m(r) \Psi^{(0)}_{m'}(r) = \delta_{mm'} \tag{2.12} \]
so that if the coefficients \(a_{\pm 1/2}\) are subjected to the constraint
\[ |a_{1/2}|^2 + |a_{-1/2}|^2 = 1, \tag{2.13} \]
the function \(\Psi^{(0)}(r)\) is normalized to unity:
\[ \int_{\mathbb{R}^3} d^3r \, \Psi^{(0)\dagger}(r) \Psi^{(0)}(r) = 1. \tag{2.14} \]
It follows from the standard Schrödinger–Rayleigh perturbation theory that the so-far unknown corrections $E^{(1)}$ and $\Psi^{(1)}(r)$ [and also the coefficients $a_{\pm 1/2}$ hidden in $\Psi^{(0)}(r)$] enter the inhomogeneous Dirac–Coulomb equation
\[
\left[-\imath\hbar \mathbf{a} \cdot \nabla + \beta mc^2 - \frac{Ze^2}{(4\pi\epsilon_0) r} - E^{(0)}\right] \Psi^{(1)}(r) = -[V_L^{(1)}(r) - E^{(1)}] \Psi^{(0)}(r),
\]
which is to be solved subject to the usual physical regularity requirements as well as the orthogonality constraints
\[
\int_{\mathbb{R}^3} \mathrm{d}^3r \, \Psi^{(0)}(r)^\dagger \Psi^{(1)}(r) = 0 \quad (m = \pm \frac{1}{2}).
\]
After Eq. (2.15) is projected onto the unperturbed basis states $\Psi^{(0)}_m(r)$, $(m = \pm \frac{1}{2})$, this yields the homogeneous algebraic system
\[
\sum_{m'=-1/2}^{1/2} \left[V_L^{(1)} - E^{(1)}\delta_{m,m'}\right] a_{m'} = 0 \quad (m = \pm \frac{1}{2}),
\]
where
\[
V_{L,m,m'}^{(1)} = \epsilon \sqrt{\frac{4\pi}{2L + 1}} \sum_{M=-L}^{L} C_{LM}^{(1)*} \int_{\mathbb{R}^3} \mathrm{d}^3r \, \Psi_m^{(0)}(r)^\dagger Y_{LM}(\mathbf{r}) \Psi_{m'}^{(0)}(r).
\]
Denoting
\[
\langle \Omega_{\kappa,m_\kappa} | Y_{LM} \Omega_{\kappa',m_{\kappa'}} \rangle \equiv \int_4 \mathrm{d}^2r_r \Omega_{\kappa,m_\kappa}(\mathbf{r}) Y_{LM}(\mathbf{r}) \Omega_{\kappa',m_{\kappa'}}(\mathbf{r})
\]
and exploiting the known identity
\[
\langle \Omega_{-\kappa,m_\kappa} | Y_{\lambda\mu} \Omega_{-\kappa',m_{\kappa'}} \rangle = \langle \Omega_{\kappa,m_\kappa} | Y_{\lambda\mu} \Omega_{\kappa',m_{\kappa'}} \rangle,
\]
we obtain
\[
V_{L,m,m'}^{(1)} = \epsilon \sqrt{\frac{4\pi}{2L + 1}} \int_{0}^{\infty} \mathrm{d}r_r r L \left\{ [P^{(0)}(r)]^2 + [Q^{(0)}(r)]^2 \right\} \sum_{M=-L}^{L} C_{LM}^{(1)*} \langle \Omega_{-m} | Y_{LM} \Omega_{-m'} \rangle.
\]
The angular integral in Eq. (2.21) may be evaluated with the aid of the known formula
\[
\sqrt{\frac{4\pi}{2L + 1}} \langle \Omega_{\kappa,m_\kappa} | Y_{LM} \Omega_{\kappa',m_{\kappa'}} \rangle = (-)^{m_\kappa + 1/2} \sqrt{\kappa\kappa'} \left( \begin{array}{c|cc} |\kappa| - \frac{1}{2} & L & |\kappa'| - \frac{1}{2} \\ \hline 0 & L - M & -M \\ \frac{1}{2} & -m_\kappa & \frac{1}{2} \end{array} \right) \Pi(l_\kappa, L, l_{\kappa'}),
\]
where \(\begin{array}{ccc} j_\kappa & j_\kappa & j_{\kappa'} \\ m_\kappa & m_\kappa & m_{\kappa'} \end{array}\) denotes Wigner’s 3j coefficient, while
\[
\Pi(l_\kappa, L, l_{\kappa'}) = \left\{ \begin{array}{ll} 1 & \text{for } l_\kappa + L + l_{\kappa'} \text{ even} \\ 0 & \text{for } l_\kappa + L + l_{\kappa'} \text{ odd} \end{array} \right.
\]
with
\[
l_\kappa = |\kappa + \frac{1}{2} - \frac{1}{2}|
\]
and similarly for $l_{\kappa'}$. One finds
\[
\langle \Omega_{-m} | Y_{LM} \Omega_{-m'} \rangle = \frac{1}{\sqrt{4\pi}} \delta_{L0} \delta_{M0} \delta_{mm'}.
\]
Since we have excluded the case \( L = 0 \) from the very beginning, we have
\[
V_{L_{mm'}}^{(1)} = 0,
\]
which implies immediately [cf. Eq. (2.17)] that for any \( L \) it holds that
\[
E^{(1)} = 0
\]
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
\[
\Psi^{(1)}(r) = -e \sqrt{\frac{4\pi}{2L + 1}} \sum_{M = -L}^{L} C_{LM}^{(1)*} \int_{\mathbb{R}^3} d^3r' \bar{G}^{(0)}(r, r')r'^LY_{LM}(n'_{r'})\Psi^{(0)}(r'),
\]
where \( \bar{G}^{(0)}(r, r') \) is the generalized (or reduced) Dirac–Coulomb Green’s function [7, Sec. 6] associated with the ground state of the atom under investigation.

3 Electric multipole moments of the atom in the multipole electric field and atomic multipole polarizabilities

3.1 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 \( \Psi(r) \), the electronic cloud of the atom may be characterized, among others, by its electric multipole moments \( Q_{\lambda} \) with the spherical components
\[
Q_{\lambda\mu} = \sqrt{\frac{4\pi}{2\lambda + 1}} \int_{\mathbb{R}^3} d^3 r r^\lambda Y_{\lambda\mu}(n_r) \rho(r),
\]
where
\[
\rho(r) = \frac{-e\Psi^\dagger(r)\Psi(r)}{\int_{\mathbb{R}^3} d^3 r' \Psi^\dagger(r')\Psi(r')}
\]
may be considered as a smeared electronic charge density. In the case the function \( \Psi(r) \) may be approximated as in Eq. (2.8), after Eqs. (2.9), (2.14) and (2.16) are taken into account, the density \( \rho(r) \) may be approximately written as
\[
\rho(r) \simeq \rho^{(0)}(r) + \rho^{(1)}(r),
\]
where
\[
\rho^{(0)}(r) = -e\Psi^{(0)*}(r)\Psi^{(0)}(r)
\]
and
\[
\rho^{(1)}(r) = -2e \text{Re}[\Psi^{(0)*}(r)\Psi^{(1)}(r)].
\]
Accordingly, Eq. (3.3) implies
\[
Q_{\lambda\mu} \simeq Q_{\lambda\mu}^{(0)} + Q_{\lambda\mu}^{(1)},
\]
where
\[
Q_{\lambda\mu}^{(0)} = -e \sqrt{\frac{4\pi}{2\lambda + 1}} \int_{\mathbb{R}^3} d^3 r \Psi^{(0)*}(r)r^\lambda Y_{\lambda\mu}(n_r)\Psi^{(0)}(r)
\]
and
\[
Q_{\lambda\mu}^{(1)} = -e \sqrt{\frac{4\pi}{2\lambda + 1}} \int_{\mathbb{R}^3} d^3 r [\Psi^{(0)*}(r)\Psi^{(1)}(r) + \Psi^{(1)*}(r)\Psi^{(0)}(r)]
\]
\footnote{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.}
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. 2, it is easy to show that the only non-vanishing multipole moment of the atom in the unperturbed ground state is the monopole one:

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

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

With the aid of the identity

\[
Y_{\lambda \mu}(\mathbf{n}_r) = (-)^{\lambda}Y^{*}_{\lambda-\mu}(\mathbf{n}_r) \tag{3.10}
\]

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

\[
Q^{(1)}_{\lambda \mu} = \tilde{Q}^{(1)}_{\lambda \mu} + (-)^{\lambda} \tilde{Q}^{(1)*}_{\lambda-\mu}, \tag{3.11}
\]

with

\[
\tilde{Q}^{(1)}_{\lambda \mu} = 4\pi e^2 \frac{\sqrt{2L+1}}{\pi^2} \sum_{\lambda=-L}^{L} C^{(1)*}_{LM} \times \int_{\mathbb{R}^3} d^3r \int_{\mathbb{R}^3} d^3r' \Psi(0)(\mathbf{r}) \mathbf{r}^{\lambda} Y_{\lambda \mu}(\mathbf{n}_r) \mathcal{G}^{(0)}(\mathbf{r}, \mathbf{r'}) \mathbf{r}^{L} Y_{LM}(\mathbf{n}_r') \Psi(0)(\mathbf{r'}). \tag{3.12}
\]

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’s function \(\mathcal{G}^{(0)}(\mathbf{r}, \mathbf{r'})\):

\[
\mathcal{G}^{(0)}(\mathbf{r}, \mathbf{r'}) = \frac{4\pi e^2}{\epsilon^2} \sum_{|\lambda|=\infty} \sum_{m_\lambda=-|\lambda|+1/2}^{1/2} \frac{1}{r^{\lambda}} \begin{pmatrix}
  g^{(0)}_{(+\lambda)m}(r, r') \Omega_{\lambda m}(\mathbf{n}_r) \Omega_{\lambda m}^\dagger(\mathbf{n}_r') & -i g^{(0)}_{(-\lambda)m}(r, r') \Omega_{\lambda m}(\mathbf{n}_r) \Omega_{\lambda m}^\dagger(\mathbf{n}_r') \\
  i g^{(0)}_{(+\lambda)m}(r, r') \Omega_{-\lambda m}(\mathbf{n}_r) \Omega_{-\lambda m}^\dagger(\mathbf{n}_r') & g^{(0)}_{(-\lambda)m}(r, r') \Omega_{-\lambda m}(\mathbf{n}_r) \Omega_{-\lambda m}^\dagger(\mathbf{n}_r')
\end{pmatrix}. \tag{3.13}
\]

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

\[
\tilde{Q}^{(1)}_{\lambda \mu} = (4\pi e^2) \frac{4\pi}{\sqrt{2L+1}} \sum_{\lambda=-L}^{L} \sum_{m_\lambda=-|\lambda|+1/2}^{1/2} \sum_{m'=1/2}^{1/2} \sum_{m''=-1/2}^{1/2} a^*_{m} a_{m'} C^{(1)*}_{LM} \langle \Omega_{-1m} | Y_{\lambda \mu} \Omega_{\lambda m} \rangle \langle \Omega_{\lambda m'} | \mathcal{G}^{(0)}_{LM} \Omega_{-1m''} \rangle, \tag{3.14}
\]

where \(R^{(L_1, L_2)}_{\lambda\mu}(P(0), Q^{(0)}; P(0), Q^{(0)})\) is a particular case of a general double radial integral

\[
R^{(L_1, L_2)}_{\lambda\mu}(F_a, F_b; F_c, F_d) = \int_0^\infty dr \int_0^\infty dr' \left( F_a(r) F_b(r') \right) r^{L_1} \mathcal{G}^{(0)}_{\lambda \mu}(r, r') r^{L_2} \left( F_c(r') F_d(r) \right). \tag{3.15}
\]

(other particular forms of this integral will appear in Secs. 4 to 8), with the matrix

\[
\mathcal{G}^{(0)}_{\lambda \mu}(r, r') = \begin{pmatrix}
  g^{(0)}_{(+\lambda)m}(r, r') & g^{(0)}_{(-\lambda)m}(r, r') \\
  g^{(0)}_{(+\lambda)m}(r', r) & g^{(0)}_{(-\lambda)m}(r', r')
\end{pmatrix}. \tag{3.16}
\]
being the radial generalized Dirac–Coulomb Green’s function associated with the ground-state atomic energy level (2.6). The two angular integrals in Eq. (5.14) 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 \( m_\kappa, m \) and \( m' \). After straightforward, though tedious, calculations, one finds that the only non-vanishing contributions to \( \tilde{Q}_{\lambda \mu} \) come from the terms with \( \kappa = L \) and \( \kappa = -L - 1 \); one has

\[
\tilde{Q}_{\lambda \mu}^{(1)} = \tilde{Q}_{\lambda \mu, L}^{(1)} + \tilde{Q}_{\lambda \mu, -L-1}^{(1)},
\]

with

\[
\tilde{Q}_{\lambda \mu, \kappa}^{(1)} = \delta_{\lambda L} (4\pi\epsilon_0) \frac{\text{sgn}(\kappa)}{(2L+1)^2} R_{\kappa}^{L,L}(P^{(0)}, Q^{(0)}; P^{(0)}, Q^{(0)}) \left\{ [\kappa + \mu(|a_{1/2}|^2 - |a_{-1/2}|^2)] C_{L\mu}^{(1)} + \sqrt{(L - \mu)(L + \mu + 1)} a_{1/2} a_{-1/2} C_{L,\mu+1}^{(1)} \right\} + \sqrt{(L - \mu)(L + \mu + 1)} a_{1/2} a_{-1/2} C_{L,\mu-1}^{(1)} \right\} \quad (\kappa = L, -L - 1).
\]

The asterisks at the components of the tensor \( C_{L}^{(1)} \) 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 \( \tilde{Q}_{\lambda \mu}^{(1)} \) in the form

\[
\tilde{Q}_{\lambda \mu}^{(1)} = \tilde{Q}_{\lambda \mu}^{(1)} \delta_{\lambda L},
\]

with

\[
\tilde{Q}_{L,\mu}^{(1)} = \tilde{Q}_{L,\mu, L}^{(1)} + \tilde{Q}_{L,\mu, -L-1}^{(1)},
\]

where

\[
\tilde{Q}_{L,\mu, \kappa}^{(1)} = (4\pi\epsilon_0) \frac{2|\kappa|}{(2L+1)^2} R_{\kappa}^{L,L}(P^{(0)}, Q^{(0)}; P^{(0)}, Q^{(0)}) C_{L,\mu}^{(1)} \quad (\kappa = L, -L - 1).
\]

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

\[
Q_{\lambda} \simeq Q_{\lambda}^{(0)} \delta_{\lambda 0} + Q_{\lambda}^{(1)} \delta_{\lambda L}.
\]

### 3.2 Atomic multipole polarizabilities

The \( 2^L \)-pole polarizability of the atom in the ground state, \( \alpha_{EL \rightarrow EL} \), is defined as a proportionality factor between the induced electric multipole moment \( Q_{L}^{(1)} \) and the field tensor \( C_{L}^{(1)} \) appearing in the expression (2.1) for the perturbing \( 2^L \)-pole electric potential

\[
Q_{L}^{(1)} = (4\pi\epsilon_0) \alpha_{EL \rightarrow EL} C_{L}^{(1)}
\]

(the SI factor \( 4\pi\epsilon_0 \) has been separated out in order to secure that the physical dimension of \( \alpha_{EL \rightarrow EL} \) is \( 2^{L+1} \), where \( L \) stands for length). It follows from Eqs. (3.23) and (3.24)–(3.24) that the polarizability \( \alpha_{EL \rightarrow EL} \), hereafter denoted in the standard manner as \( \alpha_L \), may be written as the sum

\[
\alpha_L = \alpha_{L, L} + \alpha_{L, -L-1},
\]

with the constituents being given by

\[
\alpha_{L, \kappa} = \frac{2|\kappa|}{(2L+1)^2} R_{\kappa}^{L,L}(P^{(0)}, Q^{(0)}; P^{(0)}, Q^{(0)}) \quad (\kappa = L, -L - 1).
\]

\(^4\) The multipole polarizability \( \alpha_L \) may be equivalently defined through the formula \( E^{(2)} = -\frac{1}{\epsilon_0} \frac{2}{(2L+1)^2} \alpha_L C_{L}^{(1)} \cdot C_{L}^{(1)} \), where \( E^{(2)} \) is the second-order correction to energy. The reader is referred to Appendix A for the justification of this statement.
The remaining task is to evaluate the double radial integral \( R^{LL}_\kappa (P^{(0)}, Q^{(0)}; P^{(0)}, Q^{(0)}) \). This will be done below with the aid of the Sturmian expansion of the radial generalized Dirac–Coulomb level (2.6) [here \( L \) are the radial Dirac–Coulomb Sturmian functions associated with the atomic ground-state energy and \( \kappa \) is the pertinent Sturmian eigenvalue. The “apparent principal quantum number” appearing in \( n \), 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 \( N_{\kappa} = -\kappa \).

Substitution of the expansion (3.26) into the definition of the double radial integral which appears in Eqs. (3.27) and (3.28) is defined as

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

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 \( N_{\kappa} = -\kappa \).

Substitution of the expansion (3.26) into the definition of the double radial integral which appears in Eq. (3.27) yields \( \alpha_{L,\kappa} \) in the form

\[
\alpha_{L,\kappa} = \frac{2|\kappa|}{(2L+1)!} \sum_{n_r=\infty}^{\infty} \frac{1}{\mu_{n_r,\kappa}} - 1 \int_0^\infty dr \, r^L \frac{d}{dr} \left[ P^{(0)}(r) S^{(0)}_{n_r,\kappa}(r) + Q^{(0)}(r) T^{(0)}_{n_r,\kappa}(r) \right] 
\]

\[
\times \int_0^\infty dr' \, r'^L \left[ \mu_{n_r,\kappa} P^{(0)}(r') S^{(0)}_{n_r,\kappa}(r') + Q^{(0)}(r') T^{(0)}_{n_r,\kappa}(r') \right] \quad (\kappa = L, -L - 1). 
\]

The evident disadvantage 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), (2.27), (2.28), the integral formula \( \beta x \) Eq. (7.414.11)]

\[
\int_0^\infty d\rho \, \rho^\gamma e^{-\rho} L_n^{(\alpha)}(\rho) = \frac{\Gamma(\gamma + 1)\Gamma(n + \alpha - \gamma)}{n!\Gamma(\alpha - \gamma)} \quad (\text{Re } \gamma > -1) 
\]

and the identity

\[
\gamma_\kappa^2 = \gamma_1^2 + \kappa^2 - 1, 
\]

one finds that

\[
\int_0^\infty dr \, r^L \left[ P^{(0)}(r) S^{(0)}_{n_r,\kappa}(r) + Q^{(0)}(r) T^{(0)}_{n_r,\kappa}(r) \right] 
\]

\[
= - \frac{a_0}{2} \left( \frac{L!}{\sqrt{2|n_r| + \gamma_\kappa}^2 + (\alpha Z)^2} \right) \left( \frac{\Gamma(\gamma_\kappa + 1 + L + 1)!\Gamma(\gamma_\kappa + \gamma_1 + 1 - L - 1)!}{\Gamma(\gamma_\kappa + \gamma_1 + 1)!\Gamma(\gamma_\kappa + \gamma_1)!} \right) 
\]

\[
\times \left[ \gamma_1 (N_{n_r,\kappa} + \kappa) - (|n_r| + \gamma_\kappa - \gamma_1 - L - 1) \right] 
\]

\[
\times \left[ \gamma_\kappa (N_{n_r,\kappa} + \kappa) - (|n_r| + \gamma_\kappa + \gamma_1 - 1 - L) \right] 
\]

\[
\times \left[ \gamma_\kappa (N_{n_r,\kappa} + \kappa) - (|n_r| + \gamma_\kappa - \gamma_1 - L - 1) \right] 
\]

(3.33)
The two series in Eq. (3.35) may be expressed in terms of the generalized hypergeometric function 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 \(\alpha_{L,\kappa}\):

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

The two series in Eq. (3.35) may be expressed in terms of the generalized hypergeometric function \(\,\!_{3}F_{2}\) of the unit argument. With the aid of the identity

\[
\sum_{n=0}^{\infty} \frac{\Gamma(n+a_1)\Gamma(n+a_2)\Gamma(n+a_3)}{n!\Gamma(n+b_1)\Gamma(n+b_2)} = \frac{\Gamma(a_1)\Gamma(a_2)\Gamma(a_3)}{\Gamma(b_1)\Gamma(b_2)} \,\!_{3}F_{2}\left(\begin{array}{c}
a_1, a_2, a_3 \\
b_1, b_2, b_3
\end{array} ; 1\right) \quad [\text{Re}(b_1 + b_2 - a_1 - a_2 - a_3) > 0], \tag{3.36}
\]

one arrives at

\[
\alpha_{L,\kappa} = \frac{a_0^{2L+1}}{Z^{2L+2}} \frac{|\kappa| \Gamma^2(\gamma_\kappa + \gamma_1 + L + 1)}{2L(2L+1) \Gamma(2\gamma_1 + 1) \Gamma(2\gamma_\kappa + 1)} \times \left\{ \frac{\gamma_1 [\gamma_1(\kappa + 1) + 2(\kappa + 1)]}{\gamma_\kappa - \gamma_1 + 1} \,\!_{3}F_{2} \left(\begin{array}{c}
\gamma_\kappa - \gamma_1 - L, \gamma_\kappa - \gamma_1 - L, \gamma_\kappa - \gamma_1 + 1 \\
\gamma_\kappa - \gamma_1 + 1, 2\gamma_\kappa + 1
\end{array} ; 1\right) - \frac{\gamma_\kappa + \gamma_1}{\kappa + 1} \,\!_{3}F_{2} \left(\begin{array}{c}
\gamma_\kappa - \gamma_1 - L, \gamma_\kappa - \gamma_1 - L, \gamma_\kappa - \gamma_1 + 1 \\
\gamma_\kappa - \gamma_1 + 1, 2\gamma_\kappa + 1
\end{array} ; 1\right) \right\} \quad (\kappa = L, -L - 1). \tag{3.37}
\]

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

\[
\,\!_{3}F_{2}\left(\begin{array}{c}
a_1, a_2, a_3 \\
a_3 + 1, b, b + 1
\end{array} ; 1\right) = \frac{\Gamma(b)\Gamma(b-a_1-a_2+1)}{(b-a_3+1)\Gamma(b-a_1)\Gamma(b-a_2)} - \frac{(a_1-a_3-1)(a_2-a_3-1)(a_3+1)(b-a_3-1)}{(a_3+1)(b-a_3)} \,\!_{3}F_{2} \left(\begin{array}{c}
a_1, a_2, a_3 + 1 \\
a_3 + 2, b, b + 1
\end{array} ; 1\right) \quad [\text{Re}(b-a_1-a_2) > -1], \tag{3.38}
\]

which may be used to eliminate one of the two \(\,\!_{3}F_{2}\)'s in favor of the other. It appears that a bit more compact result is obtained if the first \(\,\!_{3}F_{2}\)'s (1) is retained:

\[
\alpha_{L,\kappa} = \frac{a_0^{2L+1}}{Z^{2L+2}} \frac{|\kappa| \Gamma(2\gamma_1 + 2L + 2)}{2L(2L+1) \Gamma(2\gamma_1 + 1) \Gamma(2\gamma_\kappa + 1)} \times \left\{ \frac{\gamma_1 [\gamma_1(\kappa + 1) + L + 1]^{2} \Gamma^2(\gamma_\kappa + \gamma_1 + L + 1)}{(\gamma_\kappa - \gamma_1 + 1) \Gamma(2\gamma_1 + 2L + 2) \Gamma(2\gamma_\kappa + 1)} - 1 \right\} \quad (\kappa = L, -L - 1). \tag{3.39}
\]
Specializing to the two admitted values of $\kappa$, we finally arrive at
\[ \alpha_{L,L} = a_0^{2L+1} \frac{L! (2\gamma_1 + 2L + 2)}{Z^{2L+2} 2^{2L}(L+1)(2L+1) \Gamma(2\gamma_1+1)} \times 3 F_2 \left( \Gamma(\gamma_1 - L, \gamma_L, \gamma_L - 1, \gamma_L - 1, 1 \right), 1) \],
(3.40a)

and
\[ \alpha_{L,-L-1} = a_0^{2L+1} \frac{(L+1)! (2\gamma_1 + 2L + 2)}{Z^{2L+2} 2^{2L} L(2L+1) \Gamma(2\gamma_1+1)} \times 3 F_2 \left( \Gamma(\gamma_1 - L, \gamma_L, \gamma_L - 1, \gamma_L - 1, 1 \right), 1) \],
(3.40b)

respectively. Hence, the closed-form expression for the $2L$-pole polarizability of the hydrogen-like in the ground state is
\[ \alpha_L = a_0^{2L+1} \frac{L! (2\gamma_1 + 2L + 2)}{Z^{2L+2} 2^{2L} L(2L+1)(2L+1) \Gamma(2\gamma_1+1)} \times \left\{ 1 + \frac{L^2(L+1)^2(\gamma_L + 1)^2}{(2L+1)(\gamma_L + 1) \Gamma(2\gamma_1 + 2L + 2) \Gamma(2\gamma_L + 1)} \times 3 F_2 \left( \Gamma(\gamma_1 - L, \gamma_L, \gamma_L - 1, \gamma_L - 1, 1 \right), 1) \right\}.
(3.41)

In the dipole case ($L = 1$), Eq. (3.11) yields
\[ \alpha_1 = a_0^{2L+1} \frac{(\gamma_1 + 1)(2\gamma_1 + 1)(4\gamma_2^2 + 13\gamma_2 + 12)}{36} \times 3 F_2 \left( \Gamma(\gamma_2 - 1, \gamma_2 - 1, \gamma_2 - 1, \gamma_2 - 1, 1 \right), 1) \],
(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 (3.11), are presented in Table II. Calculations have been done for two values of the inverse of the fine-structure constant: $\alpha^{-1} = 137.035 999 139$ (from CODATA 2014) and $\alpha^{-1} = 137.035 999 074$ (from CODATA 2010), in the latter case to enable making comparison with data available in Refs. [21][22]. Table II confirms almost perfect numerical accuracy of results obtained computationally by Tang et al. [21] using the $B$-spline Galerkin method, and also high quality of numbers generated by Filippin et al. [22] with the use of the Langrange-mesh method.

Tabulation of exact numerical values of the first four multipole polarizabilities for ground states of selected hydrogenic ions is presented in Table III. Again two data sets are displayed, as a result of the use of the two aforementioned values of the inverse of the fine-structure constant. In general, the present data generated with the CODATA 2010 value of $\alpha^{-1}$ 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].

In the final step, we shall provide an approximate formula for the polarizability $\alpha_L$ that is correct to the second order in $\alpha Z$. Using
\[ \gamma_\kappa \simeq |\kappa| \left( \frac{\alpha Z^2}{2|\kappa|} \right), \]
(3.43)
where
\[ \psi(z) = \frac{1}{\Gamma(z)} \frac{d\Gamma(z)}{dz} \]  
(3.45)
is the digamma function, one finds
\[ _3F_2 \left( \begin{array}{c} \gamma_L - \gamma_1 - L, \gamma_L - \gamma_1 - 1, \gamma_L + 1 \\ \gamma_L - \gamma_1 + 2, \gamma_L + 1 \end{array} ; 1 \right) \]
\[ \simeq \frac{2L^2 + 4L + 1}{(L + 1)(2L + 1)} - (\alpha Z)^2 \frac{4L^4 + 2L^3 - 8L^2 - 3L + 1}{2L(2L + 1)^2} \]  
(3.46)
and
\[ _3F_2 \left( \begin{array}{c} \gamma_{L+1} - \gamma_1 - L, \gamma_{L+1} - \gamma_1 - 1, \gamma_{L+1} + 1 \\ \gamma_{L+1} - \gamma_1 + 2, 2\gamma_{L+1} + 1 \end{array} ; 1 \right) \simeq 1, \]  
(3.47)
and further
\[ \alpha_{L,L} \simeq \frac{a_0^{2L+1}}{2^{2L+2}} \frac{(L + 2)(2L)!}{2L} \left\{ 1 - (\alpha Z)^2 \left[ \psi(2L + 3) - \psi(3) + \frac{2L^5 + 7L^4 + 6L^3 - L - 1}{L(2L + 1)(2L + 2)} \right] \right\}, \]  
(3.48a)
\[ \alpha_{L,L-1} \simeq \frac{a_0^{2L+1}}{2^{2L+2}} \frac{(L + 1)(L + 2)(2L - 1)!}{2^{2L-1}} \times \left\{ 1 - (\alpha Z)^2 \left[ \psi(2L + 3) - \psi(3) + \frac{4L^3 + 10L^2 + 7L + 2}{2L(2L + 1)^2} \right] \right\}. \]  
(3.48b)
Adding Eqs. (3.48a) and (3.48b) yields the following approximation for \( \alpha_L \):
\[ \alpha_L \simeq \frac{a_0^{2L+1}}{2^{2L+1}} \frac{(L + 2)(2L + 1)!}{2^{2L+2}} \frac{1}{L} \times \left\{ 1 - (\alpha Z)^2 \left[ \psi(2L + 3) - \psi(3) + \frac{4L^5 + 18L^4 + 22L^3 + 7L^2 - 2}{2L(2L + 1)^2} \right] \right\}, \]  
(3.49)
which is identical with the one given in Refs. [14][16] and may be also shown to be equivalent to the counterpart expressions given in Ref. [17] and an erratum to Ref. [18]. If in the above equation one uses recursively the relation
\[ \psi(z + 1) = \psi(z) + \frac{1}{z}, \]  
(3.50)
a bit more compact approximation to \( \alpha_L \) is obtained:
\[ \alpha_L \simeq \frac{a_0^{2L+1}}{2^{2L+2}} \frac{(L + 2)(2L + 1)!}{2^{2L+2}} \times \left\{ 1 - (\alpha Z)^2 \left[ \psi(2L) - \psi(2) + \frac{14L^3 + 43L^2 + 40L + 15}{2L(2L + 1)^2} \right] \right\}. \]  
(3.51)
Explicit expressions for the quasi-relativistic approximations to \( \alpha_L \) with 1 \( \leq L \leq 4 \), resulting from Eq. (3.51), are displayed in Table III

[Place for Table III]
4 Magnetic multipole moments of the atom in the multipole electric field and atomic $\mathbf{E}L \rightarrow M(L \mp 1)$ multipole cross-susceptibilities

4.1 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 $\mathbf{M}$ for a stationary sourceless current distribution $j(r)$ are defined as

$$\mathcal{M}_{\lambda\mu} = -i \sqrt{\frac{4\pi\lambda}{(\lambda + 1)(2\lambda + 1)}} \int_{\mathbb{R}^3} d^3r \, r^\lambda Y_{\lambda\mu}(n_r) \cdot j(r), \quad (4.1)$$

where $Y_{\lambda\mu}(n_r)$ is a particular vector spherical harmonic [38, Sec. 7.3.1]. The right-hand side of Eq. (4.1) may be transformed to another form using the identity [38, Sec. 7.3.1]

$$Y_{\lambda\mu}(n_r) = \Lambda Y_{\lambda\mu}(n_r) \sqrt{\frac{\lambda}{\lambda + 1}}, \quad (4.2)$$

where

$$\Lambda = -ir \times \nabla \quad (4.3)$$

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

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

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

$$j(r) = -\frac{i}{2\lambda + 1} \int_{\mathbb{R}^3} d^3r' \, \psi^\dagger(r') \psi(r') \quad (4.5)$$

may be approximated as

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

where

$$j^{(0)}(r) = -\frac{i}{2\lambda + 1} \psi^\dagger(0)(r) \alpha \psi(0)(r) \quad (4.7)$$

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

$$j^{(1)}(r) = -2e \text{Re}[\psi^\dagger(0)(r) \alpha \psi(1)(r)] \quad (4.8)$$

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

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

where

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

are components of the magnetic $2^L$-pole moment of the atom in the unperturbed state $\psi(0)(r)$, while

$$\mathcal{M}_{\lambda\mu}^{(1)} = i \sqrt{\frac{4\pi}{2\lambda + 1}} \int_{\mathbb{R}^3} d^3r \, r^\lambda Y_{\lambda\mu}(n_r) \Lambda \cdot j^{(1)}(r) \quad (4.11)$$
is the first-order field-induced correction to \( \mathcal{M}_{\lambda \mu}^{(0)} \).

It has been shown by us in Ref. [23] that the only non-vanishing unperturbed multipole moment \( \mathbf{M}_{\lambda}^{(0)} \) is the dipole one:

\[
\mathcal{M}_{\lambda \mu}^{(0)} = \mathcal{M}_{\lambda \mu}^{(0)} \delta_{\lambda 1},
\]

(4.12)

the spherical components of which are

\[
\begin{align*}
\mathcal{M}_{1,0}^{(0)} &= -\frac{1}{3} (2\gamma + 1) \mu_B \left(|a_{1/2}|^2 - |a_{-1/2}|^2\right), \\
\mathcal{M}_{1,\pm1}^{(0)} &= \pm \frac{\sqrt{2}}{3} (2\gamma + 1) \mu_B a_{\pm1/2}^* a_{\mp1/2},
\end{align*}
\]

(4.13a,b)

where

\[
\mu_B = \frac{\hbar}{2m_e}
\]

(4.14)

is the Bohr magneton. If we introduce the unit vector \( \mathbf{\nu} \) with the cyclic components

\[
\nu_0 = |a_{1/2}|^2 - |a_{-1/2}|^2, \quad \nu_{\pm1} = \mp \sqrt{2} a_{\pm1/2}^* a_{\mp1/2},
\]

(4.15)

the magnetic dipole moment vector may be compactly written as

\[
\mathbf{M}_1^{(0)} = -\frac{2\gamma + 1}{3} \mu_B \mathbf{\nu}.
\]

(4.16)

The parametrization

\[
a_{1/2} = e^{-i(\chi+\phi)/2} \cos(\vartheta/2), \quad a_{-1/2} = e^{-i(\chi-\phi)/2} \sin(\vartheta/2), \quad (0 \leq \chi, \phi < 2\pi, 0 \leq \vartheta \leq \pi)
\]

(4.17)

implies that

\[
\nu_0 = \cos \vartheta, \quad \nu_{\pm1} = \pm \frac{1}{\sqrt{2}} e^{\pm i\phi} \sin \vartheta,
\]

(4.18)

i.e., \( \vartheta \) and \( \phi \) may be considered as the polar and the azimuthal angles, respectively, of the vector \( \mathbf{\nu} \) in the spherical coordinate system.

Once the nature of the unperturbed moments has been explained, we proceed to the analysis of the induced moments \( \mathbf{M}_1^{(1)} \). Substituting the expression \([18]\) for the induced current into the definition \([11]\), after using the identity \([3-10]\), we obtain

\[
\mathcal{M}_{\lambda \mu}^{(1)} = \mathcal{M}_{\lambda \mu}^{(1)} + (-)^\mu \mathcal{M}_{\lambda,-\mu}^{(1)*},
\]

(4.19)

where

\[
\mathcal{M}_{\lambda \mu}^{(1)} = \frac{-i e \kappa}{\lambda + 1} \sqrt{\frac{4\pi}{2\lambda + 1}} \int_{\mathbb{R}^3} d^3 r \; r \mathbf{\Lambda} \cdot \left[ \Psi^{(0)}(r) \mathbf{\alpha} \Psi^{(1)}(r) \right].
\]

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

\[
\mathcal{M}_{\lambda \mu}^{(1)} = \frac{i e^2 \kappa}{\lambda + 1} \sqrt{\frac{4\pi}{(2\lambda + 1)(2L + 1)}} \sum_{L=-L}^{L} C_{LM}^{(1)*} \times \int_{\mathbb{R}^3} d^3 r \int_{\mathbb{R}^3} d^3 r' \; r \mathbf{\Lambda} \cdot \left[ \Psi^{(1)}(r) \mathbf{\alpha} \tilde{G}^{(0)}(r, r') \right] r' \mathbf{\Lambda} \cdot \left[ \Psi^{(0)}(r') \mathbf{\alpha} \tilde{G}^{(0)}(r, r') \right].
\]

(4.21)

A simplification occurs if one exploits the obvious identity

\[
\mathbf{\Lambda} \cdot \left[ \Psi^{(1)}(r) \mathbf{\alpha} \tilde{G}^{(0)}(r, r') \right] = -\left[ \mathbf{\alpha} \cdot \mathbf{\Lambda} \Psi^{(0)}(r) \right] \tilde{G}^{(0)}(r, r') + \Psi^{(0)}(r) \mathbf{\alpha} \cdot \mathbf{\Lambda} \tilde{G}^{(0)}(r, r'),
\]

(4.22)

the multipole expansion \([5,13]\) of the Green’s function \( \tilde{G}^{(0)}(r, r') \) and the relation \([35] \) Eq. (3.2.3)]

\[
\mathbf{\sigma} \cdot \mathbf{\Lambda} \Omega_{\kappa m_\kappa}(\mathbf{n}_r) = -(\kappa + 1) \Omega_{\kappa m_\kappa}(\mathbf{n}_r).
\]

(4.23)
This results in a separation of integrations over radial and angular variables, and one obtains

\[
\tilde{M}^{(1)}_{\lambda \mu} = \frac{(4\pi e_0)c}{\lambda + 1} \frac{4\pi}{\sqrt{(2\lambda + 1)(2L + 1)}} \sum_{k=-\infty}^{\infty} (k-1) R^{(\lambda,L)}_k(Q^{(0)}, P^{(0)}; P^{(0)}, Q^{(0)})
\]

\[
\times \sum_{M=-L}^{L} m = -[1/2 \sum_{m=-1/2}^{1/2} \sum_{m'=1/2}^{1/2} a_m^* a_{m'} C^{(1)}_{L,M}(\Omega_{-m} Y_{\lambda \mu} \Omega_{-m'}) (\Omega_{-m'} Y_{LM} \Omega_{-1 m'})
\]

\[
(4.24)
\]

where \( R^{(\lambda,L)}_k(Q^{(0)}, P^{(0)}; P^{(0)}, Q^{(0)}) \) is a particular case of the double radial integral defined in Eq. (5.15) 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 \( \tilde{M}^{(1)}_{\lambda \mu} \) does not vanish only if \( \lambda = L + 1 \), i.e.,

\[
\tilde{M}^{(1)}_{\lambda \mu} = \tilde{M}^{(1)}_{\lambda \mu} \delta_{\lambda, L-1} + \tilde{M}^{(1)}_{\lambda \mu} \delta_{\lambda, L+1}.
\]

(4.25)

In these two cases, one has

\[
\tilde{M}^{(1)}_{L-1, \mu} = -(4\pi e_0)c \frac{L-1}{L(4L^2 - 1)} R^{(L-1,L)}_L(Q^{(0)}, P^{(0)}; P^{(0)}, Q^{(0)})
\]

\[
\times \left[ -\sqrt{L^2 - \mu^2} |a_{1/2}|^2 - |a_{-1/2}|^2 |C^{(1)}_{L+1 \mu} + \sqrt{(L + \mu)(L + \mu + 1)} a_{1/2} a_{-1/2} C^{(1)}_{L,\mu+1}
\right.
\]

\[
- \sqrt{(L - \mu)(L - \mu + 1)} a_{1/2} a_{-1/2} C^{(1)}_{L,\mu-1} \right]
\]

(4.26)

and

\[
\tilde{M}^{(1)}_{L+1, \mu} = -(4\pi e_0)c \frac{1}{(2L + 1)(2L + 3)} R^{(L+1,L)}_L(Q^{(0)}, P^{(0)}; P^{(0)}, Q^{(0)})
\]

\[
\times \left[ \sqrt{(L + 1)^2 - \mu^2} |a_{1/2}|^2 - |a_{-1/2}|^2 |C^{(1)}_{L+1 \mu} + \sqrt{(L + \mu)(L + \mu + 1)} a_{1/2} a_{-1/2} C^{(1)}_{L,\mu+1}
\right.
\]

\[
- \sqrt{(L - \mu)(L - \mu + 1)} a_{1/2} a_{-1/2} C^{(1)}_{L,\mu-1} \right]
\]

(4.27)

respectively. On combining Eqs. (4.19), (4.26)–(4.27) and (4.15), we find that

\[
M^{(1)}_{\lambda \mu} = M^{(1)}_{\lambda \mu} \delta_{\lambda, L-1} + M^{(1)}_{\lambda \mu} \delta_{\lambda, L+1},
\]

(4.28)

where

\[
M^{(1)}_{L-1, \mu} = -(4\pi e_0)c \frac{2(L-1)}{L(4L^2 - 1)} R^{(L-1,L)}_L(Q^{(0)}, P^{(0)}; P^{(0)}, Q^{(0)}) \left[ -\sqrt{L^2 - \mu^2} \nu_0 C^{(1)}_{L\mu}
\right.
\]

\[
+ \sqrt{\frac{1}{2}(L + \mu)(L + \mu + 1)} \nu_{-1} C^{(1)}_{L,\mu+1} + \sqrt{\frac{1}{2}(L - \mu)(L - \mu + 1)} \nu_1 C^{(1)}_{L,\mu-1} \right]
\]

(4.29)

and

\[
M^{(1)}_{L+1, \mu} = -(4\pi e_0)c \frac{2}{(2L + 1)(2L + 3)} R^{(L+1,L)}_L(Q^{(0)}, P^{(0)}; P^{(0)}, Q^{(0)}) \left[ \sqrt{(L + 1)^2 - \mu^2} \nu_0 C^{(1)}_{L\mu}
\right.
\]

\[
+ \sqrt{\frac{1}{2}(L - \mu)(L - \mu + 1)} \nu_{-1} C^{(1)}_{L,\mu+1} + \sqrt{\frac{1}{2}(L + \mu)(L + \mu + 1)} \nu_1 C^{(1)}_{L,\mu-1} \right]
\]

(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.,

\[
M_\lambda \simeq M^{(0)}_\lambda \delta_{\lambda 1} + M^{(1)}_\lambda (\delta_{\lambda, L-1} + \delta_{\lambda, L+1}).
\]

(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 \(\lambda\) of the vector \(\mathbf{\nu}\), defined in Eq. (4.15) and characterizing the unperturbed atomic state, and the tensor \(\mathbf{C}_L^{(1)}\), characterizing the perturbing multipole electric field. According to the general theory of such products [38, Sec. 3.1.7], its components are given by

\[
\{ \mathbf{\nu} \otimes \mathbf{C}_L^{(1)} \}_{\lambda \mu} = \sum_{m=-L}^{L} \sum_{m=-1}^{L} \langle 1mLM|\lambda\mu\rangle \nu_m C_{LM}^{(1)},
\]

(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. [38, Table 8.2]) shows that the two induced magnetic moments \(\mathbf{M}_{L+1}^{(1)}\), components of which are displayed in Eqs. (4.29) and (4.30), may be compactly written as

\[
\mathbf{M}_{\lambda}^{(1)} = -(4\pi\epsilon_0)c \left( \frac{2\sqrt{2}}{\lambda + 1} \right) \left( \frac{L + \lambda + 1}{2(L + 1)} \right) R^{(\lambda,L)}_{\kappa\lambda}(Q^{(0)},P^{(0)},P^{(0)},Q^{(0)}) \{ \mathbf{\nu} \otimes \mathbf{C}_L^{(1)} \}_{\lambda}
\]

(\(\lambda = L \pm 1\)),

(4.33)

with

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

(4.34)

### 4.2 Atomic multipole \(\textbf{EL} \rightarrow \textbf{M}(L \pm 1)\) cross-susceptibilities

We define the atomic electric-to-magnetic multipole cross-susceptibilities \(\alpha_{\text{EL} \rightarrow \text{M}(L \pm 1)}\) through the relation

\[
\mathbf{M}_{\lambda}^{(1)} = (4\pi\epsilon_0)c \alpha_{\text{EL} \rightarrow \text{M}} \{ \mathbf{\nu} \otimes \mathbf{C}_L^{(1)} \}_{\lambda} \langle 10L0|\lambda0 \rangle
\]

(\(\lambda = L \pm 1\)),

(4.35)

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

\[
\langle 10L0|\lambda0 \rangle = (\lambda - L) \sqrt{\frac{\lambda + L + 1}{2(L + 1)}}
\]

(\(\lambda = L \pm 1\)).

(4.36)

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

\[
\alpha_{\text{EL} \rightarrow \text{M}} = -\frac{2\lambda(\lambda - L)}{(2\lambda + 1)(2L + 1)} R^{(\lambda,L)}_{\kappa\lambda}(Q^{(0)},P^{(0)},P^{(0)},Q^{(0)}) \{ \mathbf{\nu} \otimes \mathbf{C}_L^{(1)} \}_{\lambda}
\]

(\(\lambda = L \pm 1\)).

(4.37)

To tackle the latter, we exploit the Sturmian expansion (4.20), obtaining

\[
\alpha_{\text{EL} \rightarrow \text{M}} = -\frac{2\lambda(\lambda - L)}{(2\lambda + 1)(2L + 1)} \sum_{n_{\gamma}=-\infty}^{\infty} \frac{1}{\mu_{n_{\gamma}\lambda}} \int_0^\infty dr r^\lambda \left[ Q^{(0)}(r)S^{(0)}_{n_{\gamma}\lambda}(r) + P^{(0)}(r)T^{(0)}_{n_{\gamma}\lambda}(r) \right]
\]

\[
\times \int_0^\infty dr' r'^L \left[ \mu_{n_{\gamma}\lambda} P^{(0)}(r')S^{(0)}_{n_{\gamma}\lambda}(r') + Q^{(0)}(r')T^{(0)}_{n_{\gamma}\lambda}(r') \right]
\]

(\(\lambda = L \pm 1\)).

(4.38)

The second of the two, now separated, radial integrals in Eq. (4.38) is seen to be identical with the one we have evaluated in Eq. (3.34), while the first integral, with the aid of Eqs. (2.111), (3.24) and (3.31), is found to be

\[
\int_0^\infty dr r^\lambda \left[ Q^{(0)}(r)S^{(0)}_{n_{\gamma}\lambda}(r) + P^{(0)}(r)T^{(0)}_{n_{\gamma}\lambda}(r) \right]
\]

\[
= -\frac{\sqrt{2}(N_{n_{\gamma}\lambda} - \kappa_{\lambda})}{\sqrt{a_0}|n_r|N_{n_{\gamma}\lambda}(N_{n_{\gamma}\lambda} - \kappa_{\lambda})^1(2_{\gamma} + 1)^1(1 + 2_{\gamma} + 1) + 1} \times \frac{\Gamma(\gamma_{\lambda} + \gamma_1 + \lambda + 1)\Gamma(|n_r| + \gamma_{\lambda} - \gamma_1 - \lambda)}{\Gamma(\gamma_{\lambda} - \gamma_1 - \lambda)}.
\]

(4.39)
Plugging Eqs. (4.39) and (4.41) into Eq. (4.38), then transforming the resulting series \( \sum_{n=0}^{\infty} (\cdots) \) into a one of the sort \( \sum_{n=-\infty}^{\infty} (\cdots) \), and identifying subsequently the two \( 3F_2(1) \) functions, yields the cross-susceptibility \( \alpha_{EL\rightarrow MA} \) in the form

\[
\alpha_{EL\rightarrow MA} = \frac{\alpha_0^{\lambda+L+1}}{Z^{\lambda+L+1}} \frac{\lambda(\lambda - L)\Gamma(2\gamma_1 + 2\gamma_2 + 2)}{(2\gamma_1 + 1)(2\gamma_1 + 2\gamma_2 + 2)(2\gamma_1 + L + 1)} \times \left[ \frac{\gamma_1(\lambda + 1)}{\gamma_2 - \gamma_1 + 1} \right] \sum_{n=0}^{\infty} (\cdots) \quad (\lambda = L \mp 1). \tag{4.40}
\]

Eliminating the second \( 3F_2(1) \) in favor of the first one with the help of Eq. (4.38), we finally arrive at the following general expression for the cross-susceptibility in question:

\[
\alpha_{EL\rightarrow MA} = \frac{\alpha_0^{\lambda+L+1}}{Z^{\lambda+L+1}} \frac{\lambda(\lambda - L)\Gamma(2\gamma_1 + 2\gamma_2 + 2)}{(2\gamma_1 + 1)(2\gamma_1 + 2\gamma_2 + 2)(2\gamma_1 + L + 1)} \times \left[ \frac{1}{\gamma_2 - \gamma_1} \right] \sum_{n=0}^{\infty} (\cdots) \quad (\lambda = L \mp 1), \tag{4.41}
\]

where, we recall, \( \gamma_2 \) has been defined in Eq. (4.34). If in the above formula the explicit values of \( \lambda \) and \( \gamma_2 \) are set, this gives explicitly

\[
\alpha_{EL\rightarrow M(L-1)} = \frac{\alpha_0^{2L}}{Z^{2L}} \frac{(L - 1)\Gamma(2\gamma_1 + 2\gamma_2 + 2)}{(2\gamma_1 + 1)(2\gamma_1 + 2\gamma_2 + 2)(2\gamma_1 + L + 1)} \times \left[ \frac{1}{\gamma_2 - \gamma_1} \right] \sum_{n=0}^{\infty} (\cdots) \tag{4.42}
\]

and

\[
\alpha_{EL\rightarrow M(L+1)} = \frac{\alpha_0^{2L+2}}{Z^{2L+2}} \frac{(L + 1)\Gamma(2\gamma_1 + 2\gamma_2 + 2)}{(2\gamma_1 + 1)(2\gamma_1 + 2\gamma_2 + 2)(2\gamma_1 + L + 1)} \times \left[ \frac{1}{\gamma_2 - \gamma_1} \right] \sum_{n=0}^{\infty} (\cdots) \tag{4.43}
\]

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

\[
\alpha_{E1\rightarrow M2} = \frac{\alpha_0^4}{Z^4} \frac{\Gamma(2\gamma_1 + 5)}{60\Gamma(2\gamma_1 + 1)} \left[ 1 + \frac{3(\gamma_2 - \gamma_1 + 1)\Gamma(2\gamma_1 + 2)}{\gamma_2 - \gamma_1 + 1} \right] \sum_{n=0}^{\infty} (\cdots) \tag{4.44}
\]

With the use of the relation (4.38), the latter formula may be transformed into the following one:

\[
\alpha_{E1\rightarrow M2} = \frac{\alpha_0^4}{Z^4} \frac{\Gamma(2\gamma_1 + 5)}{240\Gamma(2\gamma_1 + 1)} \left[ 1 - \frac{(\gamma_2 - \gamma_1 + 1)\Gamma(2\gamma_1 + 2)}{\gamma_2 - \gamma_1 + 1} \right] \sum_{n=0}^{\infty} (\cdots) \tag{4.45}
\]

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

Numerical values of the cross-susceptibilities $\alpha_{EL \rightarrow M(L \pm 1)}$ with $1 \leq L \leq 4$ for selected hydrogenic ions, computed from Eqs. (4.42) and (4.43), are presented in Tables IV and V.

A derivation of quasi-relativistic approximations to the two cross-susceptibilities $\alpha_{EL \rightarrow M(L \pm 1)}$ is very much analogous to the procedure we have adopted in Sec. 3 for the polarizabilities $\alpha_L$. Exploiting the relations (3.43) and (3.44), one deduces the estimates

$$3 F_2 \left( \frac{\gamma_L - \gamma_1 - L}{\gamma_L - \gamma_1 + 2}, \frac{\gamma_L - \gamma_1 - 1}{2\gamma_L + 1}; 1 \right) \simeq 1 - \frac{(\alpha Z)^2}{2(L+1)(2L+1)} \frac{L-1}{2(L+2)(2L+3)}.$$  (4.46)

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

$$\alpha_{EL \rightarrow M(L-1)} \simeq \frac{\alpha a_{2L}^2}{Z^{2L}} (\alpha Z)^2 \frac{(L-1)^2(2L^3 + 5L^2 + 4L + 2)(2L - 2)!}{2^{2L}L(L+1)(2L+1)}.$$  (4.48)

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

$$\alpha_{EL \rightarrow M(L+1)} \simeq \frac{\alpha a_{2L+2}^2}{Z^{2L+2}} \frac{(L+2)(2L+2)!}{2^{2L+2}L} \times \left\{ 1 - \frac{(\alpha Z)^2}{2(L+1)^2(2L+1)(2L+2)(2L+3)} \psi(2L+4) - \psi(2) - \frac{L(2L^4 + 9L^3 + 17L^2 + 17L + 8)}{2(L+1)^2(2L+1)(2L+3)} \right\}.$$  (4.49)

It is worthwhile to notice that irrespective of the value assumed by $L$, the cross-susceptibility $\alpha_{EL \rightarrow M(L-1)}$ (hence, also the induced moment $M^{(1)}_{L-1}$) vanishes as $\alpha Z \rightarrow 0$, while in the same limit both $\alpha_{EL \rightarrow M(L+1)}$ and $M^{(1)}_{L+1}$ 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 $1 \leq L \leq 4$, are collected in Table VI.

5 Magnetic toroidal multipole moments of the atom in the multipole electric field and atomic $EL \rightarrow TL$ multipole cross-susceptibilities

5.1 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 $2^\lambda$-pole magnetic toroidal moment $T_\lambda$ due to a solenoidal current density $j(r)$ may be written in several equivalent forms, out of which for the use in this section we choose the following one:

$$T_\lambda = \frac{1}{\lambda + 1} \sqrt{\frac{4\pi}{2\lambda + 1}} \int_{\mathbb{R}^3} d^3r \, r^\lambda Y_{\lambda \mu}(n_r) r \cdot j(r).$$  (5.1)
Proceeding along the route sketched in Sec. 4 after the current is approximated as in Eq. (4.6), we obtain
\[ T_{\lambda\mu} \approx T_{\lambda\mu}^{(0)} + T_{\lambda\mu}^{(1)}, \] (5.2)
where
\[ T_{\lambda\mu}^{(0)} = \frac{1}{\lambda + 1} \sqrt{\frac{4\pi}{2\lambda + 1}} \int_{\mathbb{R}^3} d^3 r \ r^\lambda Y_{\lambda\mu}(n_r) r \cdot j^{(0)}(r) \] (5.3)
and
\[ T_{\lambda\mu}^{(1)} = \frac{1}{\lambda + 1} \sqrt{\frac{4\pi}{2\lambda + 1}} \int_{\mathbb{R}^3} d^3 r \ r^\lambda Y_{\lambda\mu}(n_r) r \cdot j^{(1)}(r), \] (5.4)
with \( j^{(0)}(r) \) and \( j^{(1)}(r) \) given, respectively, by Eqs. (4.7) and (4.8).

At first, we shall 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 \( j^{(0)}(r) \) into the right-hand side of Eq. (5.3) and then make use of Eqs. (2.9) and (2.10), together with the identity [35, Eq. (3.1.3)]
\[ n_r \cdot \sigma_{\kappa m}(n_r) = -\sigma_{-\kappa m}(n_r), \] (5.5)
obtaining
\[ T_{\lambda\mu}^{(0)} = \frac{iec}{\lambda + 1} \sqrt{\frac{4\pi}{2\lambda + 1}} \int_0^\infty dr \ r^{\lambda+1} P^{(0)}(r) Q^{(0)}(r) \times \sum_{m=-1/2}^{1/2} \sum_{m'=-1/2}^{1/2} a_m^* a_{m'} \left[ \langle \Omega_{-1m} | Y_{\lambda\mu} \Omega_{-1m'} \rangle - \langle \Omega_{1m} | Y_{\lambda\mu} \Omega_{1m'} \rangle \right]. \] (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 \( \lambda, \mu, m \) 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
\[ T_{\lambda\mu}^{(0)} = 0. \] (5.7)

Next, we turn our attention to the first-order induced moments \( T^{(1)}_\lambda \). From Eqs. (5.4), (4.8) and (3.10), we have
\[ T_{\lambda\mu}^{(1)} = \tilde{T}_{\lambda\mu}^{(1)} + (-)^{\mu} \tilde{T}_{\lambda, -\mu}^{(1)*} \] (5.8)
with
\[ \tilde{T}_{\lambda\mu}^{(1)} = \frac{-iec}{\lambda + 1} \sqrt{\frac{4\pi}{2\lambda + 1}} \int_{\mathbb{R}^3} d^3 r \ r^{\lambda+1} Y_{\lambda\mu}(n_r) \psi^{(0)\dagger}(r)n_r \cdot \alpha \psi^{(1)}(r). \] (5.9)

Skipping details that should be already obvious to the reader who has gone through Secs. 3 and 4 we come to the inference that Eq. (5.9) may be converted into
\[ \tilde{T}_{\lambda\mu}^{(1)} = \frac{i(4\pi e_0) e}{\lambda + 1} \frac{4\pi}{\sqrt{(2\lambda + 1)(2L + 1)}} \sum_{\delta = -\infty}^{L} R_{\delta^L+1\lambda}^{(L)}(Q^{(0)}, -P^{(0)}, P^{(0)}, Q^{(0)}) \times \sum_{M=-L}^{L} \sum_{m=-1/2}^{1/2} \sum_{m'=-1/2}^{1/2} a_m^* a_{m'} C_{LM}^{(1)*}(\Omega_{-1m} | Y_{\lambda\mu} \Omega_{\kappa m'} \rangle | \Omega_{\kappa m'} | Y_{LM} \Omega_{-1m'} \rangle. \] (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. 3.1 we quickly find that
\[ T_{\lambda\mu}^{(1)} = T_{\lambda\mu}^{(1)} \delta_{\lambda L}, \] (5.11)
where

\[ \mathcal{T}^{(1)}_{L\mu} = \mathcal{T}^{(1)}_{L\mu;L} + \mathcal{T}^{(1)}_{L\mu;-L-1}, \quad (5.12) \]

with

\[ \mathcal{T}^{(1)}_{L\mu;\kappa} = (4\pi\varepsilon_0) c \left\{ \frac{2i \text{sgn}(\kappa)}{L + 1}(2L + 1)^2 R^{(L+1,L)}_\kappa \left( Q^{(0)}_\mu, -P^{(0)}_\mu; P^{(0)}_\mu, Q^{(0)}_\mu \right) + \sqrt{(L - \mu)(L + \mu + 1)} a_{1/2} a_{-1/2}^\ast \mathcal{C}^{(1)}_{L,\mu+1} + \sqrt{(L + \mu)(L - \mu + 1)} a_{1/2} a_{-1/2} \mathcal{C}^{(1)}_{L,\mu-1} \right\}, \quad (5.13) \]

In Sec. 4.1, we have succeeded to express the two induced magnetic moments \( \mathbf{M}^{(1)}_{L+1} \) in terms of certain irreducible tensor products of the vector (rank-1 tensor) \( \nu \), introduced in Eq. (4.13), and the \( 2^L \)-pole tensor \( \mathbf{C}^{(1)}_L \), 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 \( \nu \), after making use of a table of the Clebsch–Gordan coefficients [38, Table 8.2], we arrive at

\[ \mathcal{T}^{(1)}_{L\mu;\kappa} = -(4\pi\varepsilon_0) c \left\{ \frac{2i \text{sgn}(\kappa)}{L + 1}(2L + 1)^2 R^{(L+1,L)}_\kappa \left( Q^{(0)}_\mu, -P^{(0)}_\mu; P^{(0)}_\mu, Q^{(0)}_\mu \right) \nu \otimes \mathbf{C}^{(1)}_L \right\}_{L\mu}, \quad \kappa = L, -L - 1. \]

In summary, in this section we have shown that in the ground state of an isolated atom all magnetic toroidal multipole moments due to 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.,

\[ \mathbf{T}_\lambda \simeq \mathcal{T}^{(1)}_{L\lambda} \delta_{\lambda L}. \quad (5.15) \]

### 5.2 Atomic multipole \( EL \rightarrow TL \) cross-susceptibilities

We define the atomic multipole electric-to-magnetic toroidal cross-susceptibilities \( \alpha_{EL \rightarrow TL} \) according to

\[ \mathcal{T}^{(1)}_L = i(4\pi\varepsilon_0) c \alpha_{EL \rightarrow TL} \sqrt{L(L + 1)} \left\{ \nu \otimes \mathbf{C}^{(1)}_L \right\}_L. \quad (5.16) \]

Comparison of Eq. (5.16) with Eqs. (5.12) and (5.14) gives \( \alpha_{EL \rightarrow TL} \) in the form of the sum

\[ \alpha_{EL \rightarrow TL} = \alpha_{EL \rightarrow TL,L} + \alpha_{EL \rightarrow TL,-L-1}, \quad (5.17) \]

with the two addends given by

\[ \alpha_{EL \rightarrow TL,L} = -\frac{2 \text{sgn}(\kappa)}{(L + 1)(2L + 1)^2} R^{(L+1,L)}_\kappa \left( Q^{(0)}_\mu, -P^{(0)}_\mu; P^{(0)}_\mu, Q^{(0)}_\mu \right) \quad (\kappa = L, -L - 1) \quad (5.18) \]

or, by virtue of the definition (3.13) and the expansion (5.20), by

\[ \alpha_{EL \rightarrow TL,L} = -\frac{2 \text{sgn}(\kappa)}{(L + 1)(2L + 1)^2} \times \sum_{n_{\nu} = -\infty}^{\infty} \frac{1}{\mu_{n_{\nu},\kappa} - 1} \int_0^\infty dr \, r^{L+1} \left[ \mathcal{S}^{(0)}_{n_{\nu},\kappa}(r) - P^{(0)}(r) T^{(0)}_{n_{\nu},\kappa}(r) \right] \times \int_0^\infty dr' \, r'^{L} \left[ \mathcal{P}^{(0)}(r') \mathcal{S}^{(0)}_{n_{\nu},\kappa}(r') + Q^{(0)}(r') T^{(0)}_{n_{\nu},\kappa}(r') \right], \quad (\kappa = L, -L - 1). \]

\[ (5.19) \]
The integral over \( r' \) is seen to be identical to the one evaluated in Eq. (5.31), while the one over \( r \), after the use is made of Eqs. (3.27) and (3.31), is found to be

\[
\int_0^\infty dr \ r^{L+1} \left[ (Q^{(0)}(r)S^{(0)}_{n,r}(r) - P^{(0)}(r)T^{(1)}_{n_r}(r)) \right]
\]

\[
= \alpha Z \left( \frac{a_0}{2\pi} \right)^{L+2} \sum_{n_r} \sqrt{\frac{\Omega}{n_r}} \sqrt{\frac{\Omega}{n_r}} N_{n,\kappa}(N_{n,\kappa} - \kappa) \Gamma(2\gamma_1 + 1) \Gamma(2\gamma_1 + 1) \times \Gamma(\gamma_1 + \gamma_1 + L + 2) \Gamma(\gamma_1 + \gamma_1 + L + 2) \times F_2 \left( \begin{array}{c} \gamma_1 - \gamma_1 - L - 1, \gamma_1 - \gamma_1 - L, \gamma_1 - \gamma_1 + 1 \end{array} ; 1 \right)
\]

\[
\times \Gamma(\gamma_1 - \gamma_1 - L - 1). \quad (5.20)
\]

Inserting Eqs. (5.31) 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. 3.2 and 4.2 to a form involving a particular \( F_2(1) \) function, yields the following general expression for \( \alpha_{EL\rightarrow TL,\kappa} \):

\[
\alpha_{EL\rightarrow TL,\kappa} = \frac{\alpha a_0^{2L+2} \text{sgn}(\kappa) \Gamma(\gamma_1 + 1 + L + 1) \Gamma(\gamma_1 + 1 + L + 1) \Gamma(\gamma_1 + 1 + L + 2)}{2^{2L+1}(L + 1)^2(2L + 1)^2} \times F_2 \left( \begin{array}{c} \gamma_1 - \gamma_1 - L - 1, \gamma_1 - \gamma_1 - L, \gamma_1 - \gamma_1 + 1 \end{array} ; 1 \right) \right.
\]

\[
\left. \times \Gamma(\gamma_1 - \gamma_1 - L - 1). \quad (5.21) \right.
\]

Hence, we find that the cross-susceptibility \( \alpha_{EL\rightarrow TL} \) is the sum of

\[
\alpha_{EL\rightarrow TL, L} = \frac{\alpha a_0^{2L+2}}{2^{2L+1}(L + 1)^2(2L + 1)^2} \times F_2 \left( \begin{array}{c} \gamma_L - \gamma_L - L - 1, \gamma_L - \gamma_L - L, \gamma_L - \gamma_L + 1 \end{array} ; 1 \right)
\]

\[
\left. \times \Gamma(\gamma_L - \gamma_L - L - 1), \quad (5.22a) \right.
\]

and

\[
\alpha_{EL\rightarrow TL, -L-1} = \frac{\alpha a_0^{2L+2}}{2^{2L+1}(L + 1)^2(2L + 1)^2} \times F_2 \left( \begin{array}{c} \gamma_{L+1} - \gamma_{L+1} - L - 1, \gamma_{L+1} - \gamma_{L+1} - L, \gamma_{L+1} - \gamma_{L+1} + 1 \end{array} ; 1 \right)
\]

\[
\left. \times \Gamma(\gamma_{L+1} - \gamma_{L+1} - L - 1), \quad (5.22b) \right.
\]

i.e., one has

\[
\alpha_{EL\rightarrow TL} = \frac{\alpha a_0^{2L+2}}{2^{2L+1}(L + 1)^2(2L + 1)^2} \times F_2 \left( \begin{array}{c} \gamma_L - \gamma_L - L - 1, \gamma_L - \gamma_L - L, \gamma_L - \gamma_L + 1 \end{array} ; 1 \right)
\]

\[
\left. \times \Gamma(\gamma_L - \gamma_L - L - 1), \quad (5.23) \right.
\]

Tabulation of numerical values of the cross-susceptibilities \( \alpha_{EL\rightarrow TL} \) with \( 1 \leq L \leq 4 \) for selected hydrogenic ions is done in Table VII

[Place for Table VII]

In the particular case when the perturbing electric field is of dipolar \( (L = 1) \) character, the first \( F_2(1) \) series on the right-hand side of Eq. (5.23) is a terminating one and \( \alpha_{E_1\rightarrow T_1} \) appears to have the relatively simple form

\[
\alpha_{E_1\rightarrow T_1} = \frac{\alpha a_0^{2L+2}}{2^{14}} \left[ \frac{(\gamma_1 + 1)^3(2\gamma_1 + 1)}{18} + \frac{(\gamma_1 - 2)F_2(\gamma_2 + \gamma_3 + 3)}{144(\gamma_2 - \gamma_1 + 1)F_2(\gamma_2 + \gamma_1 + 1)} \right]
\]

\[
\times F_2 \left( \begin{array}{c} \gamma_2 - \gamma_1 - 2, \gamma_2 - \gamma_1 - 1, \gamma_2 - \gamma_1 + 1 \end{array} ; 1 \right)
\]

\[
(5.24) \]
The dipolar case was studied by our group a decade ago in Ref. [25], where the following representation of $\alpha_{E1\rightarrow T1}$ was derived:\[\]
\[
\alpha_{E1\rightarrow T1} = \frac{\alpha a_1}{Z^4} \left\{ (\gamma_1 + 1)(2\gamma_1 + 1)(8\gamma_1^2 + 54\gamma_1^2 + 67\gamma_1 + 18) \\
- \frac{(\gamma_1 - 2)(4\gamma_1 + 1)\Gamma^2(\gamma_2 + 1/2)}{570(\gamma_2 - \gamma_1)\Gamma(2\gamma_1 + 1)\Gamma(2\gamma_2 + 1/2)} \right\}^{3F_2} \left( \gamma_2 - \gamma_1 - 1, \gamma_2 - \gamma_1 - 1, \gamma_2 - \gamma_1 ; 1 \right).
\]

Equivalence of the expressions in Eqs. (5.24) and (5.25) may be proved with the aid of the identity
\[
3F_2 \left( a_1, a_2, a_3 \right)_{a_3 + 1, b : 1} = \left[ 1 - \frac{(a_1 - a_3 - 1)(a_2 - a_3 - 1)}{(a_1 - 1)(b - a_1)} \right] \frac{\Gamma(b - a_1 - a_2 + 1)}{(b - a_3 - 1)\Gamma(b - a_1)\Gamma(b - a_2)} \\
- \frac{(a_1 - a_3 - 1)(a_2 - a_3 - 2)(a_3 - a_1 - 1)}{(a_1 - 1)(a_3 + 1)(b - a_3 - 1)} \times 3F_2 \left( a_1 - 1, a_2, a_3 + 1 \right)_{a_3 + 2, b : 1} \text{ Re} (b - a_1 - a_2) > 1.
\]

To find a quasi-relativistic limit of the general expression for the cross-susceptibilities under study, we approximate the hypergeometric function appearing in Eq. (5.22a) with the formula
\[
3F_2 \left( \gamma_L - \gamma_1 - L - 1, \gamma_L - \gamma_1 - L, \gamma_L - \gamma_1 + 1 : 1 \right) \approx \frac{2L^2 + 5L + 1}{(L + 1)(2L + 1)} - \frac{(\alpha Z)^2}{4L(L + 1)^2(2L + 1)^2} \left( 12L^5 + 32L^4 - 15L^3 - 68L^2 - 17L + 8 \right)
\]
and the one in Eq. (5.22b) using Eq. (4.47). This yields the following estimations of the two addends in Eq. (5.17):
\[
\alpha_{E\rightarrow TL,L} \approx \frac{\alpha a_0^{2L+2}}{Z^{2L+2}} \frac{(2L + 3)(2L)!}{2^{2L}L(2L + 1)} \\
\times \left\{ 1 - (\alpha Z)^2 \left[ \psi(2L + 2) - \psi(2) - \frac{2L^6 - L^5 - 26L^4 - 31L^3 + 4L + 4}{4L(2L + 1)(L + 2)(2L^2 + 5L + 1)} \right] \right\},
\]
\[
\alpha_{E\rightarrow TL,L-1} \approx -\frac{\alpha a_0^{2L+2}}{Z^{2L+2}} \frac{(2L + 1)(2L)!}{2^{2L+1}(L + 1)(2L + 1)} \\
\times \left\{ 1 - (\alpha Z)^2 \left[ \psi(2L + 2) - \psi(2) - \frac{2L^5 + 13L^4 + 27L^3 + 18L^2 - 3L - 4}{2(L + 1)^2(2L + 3)} \right] \right\}.
\]

Adding the right-hand sides of Eqs. (5.28a) and (5.28b), after some algebra we arrive at the sought quasi-relativistic representation of $\alpha_{E\rightarrow TL}$:
\[
\alpha_{E\rightarrow TL} \approx \frac{\alpha a_0^{2L+2}}{Z^{2L+2}} \frac{(L + 2)(2L + 1)!}{2^{2L+1}L(2L + 1)} \left\{ 1 - (\alpha Z)^2 \left[ \psi(2L + 3) - \psi(2) \right] \right\} + \frac{6L^7 + 29L^6 + 49L^5 + 32L^4 - L^3 - 16L^2 - 12L - 4}{2L(2L + 1)^2(2L + 1)^2}.
\]

\[\]

5 Equation (6.25) follows from Eq. (4.32) in Ref. [25], where the expression for $\tau = \alpha_{E1\rightarrow T1}$ was presented. The reader might be surprised that setting $L = 1$ in Eqs. (6.25) and adding 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 $T_{\mu \nu}^{(1)}$ of the induced toroidal moment into a sum of two $\kappa$-dependent addends is not (and, in fact, need not to be) unique, and depends on a particular integral representations of $T_{\mu \nu}$ 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.
Table VIII collects the quasi-relativistic approximations of $\alpha_{E_L \rightarrow T_L}$ obtained from Eq. (5.29) for $1 \leq L \leq 4$.

[Place for Table VIII]

6 Near-nucleus electric multipole moments of the atom in the multipole electric field and electric multipole nuclear shielding constants

6.1 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 shall be analyzing near-field (henceforth, in view of the present context, the term near-nucleus will be 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 $R_{\lambda}$, the spherical components of which are defined to be

$$R_{\lambda \mu} = \sqrt{\frac{4\pi}{2\lambda + 1}} \int_{\mathbb{R}^3} d^3r \ r^{-\lambda-1} Y_{\lambda \mu}(n_r) \rho(r),$$

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

$$R_{\lambda \mu} \approx R^{(0)}_{\lambda \mu} + R^{(1)}_{\lambda \mu},$$

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

$$R^{(0)}_{\lambda \mu} = \sqrt{\frac{4\pi}{2\lambda + 1}} \int_{\mathbb{R}^3} d^3r \ r^{-\lambda-1} Y_{\lambda \mu}(n_r) \rho^{(0)}(r)$$

and

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

respectively.

Evaluation of both $R^{(0)}_{\lambda \mu}$ and $R^{(1)}_{\lambda \mu}$ is much simplified by the fact that angular integrations involved are identical to these encountered in Sec. 3.1, where the counterpart far-field moments $Q^{(0)}_{\lambda \mu}$ and $Q^{(1)}_{\lambda \mu}$ have been analyzed. In result, one finds that

$$R_{\lambda} \approx R^{(0)}_{\lambda} \delta_{\lambda 0} + R^{(1)}_{\lambda} \delta_{\lambda L},$$

with the non-vanishing components given by

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

and

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

where

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

In the last equation, $R^{(1)}_{L\mu, \kappa} (P^{(0)}, Q^{(0)}; P^{(0)}, Q^{(0)})$ is a particular form of the double radial integral defined in Eq. (3.11). Invoking the explicit forms (2.11) of the electronic radial functions, one immediately finds that

$$R^{(0)}_{00} = -\frac{Ze}{\alpha_0 \gamma_1}.$$
6.2 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, \(\sigma_{EL \rightarrow EL}^L\), through the relation

\[
R_L^{(1)} = (4\pi\varepsilon_0)\sigma_{EL \rightarrow EL}^L \mathcal{C}_L^{(1)}.
\] (6.10)

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

\[
\sigma_{EL \rightarrow EL} = \sigma_{EL \rightarrow EL,L} + \sigma_{EL \rightarrow EL,-L-1}.
\] (6.11)

with

\[
\sigma_{EL \rightarrow EL,\kappa} = \frac{2|\kappa|}{(2L + 1)^2} R_{\kappa}^{(-L-1,L)} (P^{(0)}(t), Q^{(0)}; P^{(0)}, Q^{(0)})(\kappa = L - L - 1),
\] (6.12)

where, by virtue of Eqs. (3.15) and (3.20), the double radial integral may be written as

\[
R_{\kappa}^{(-L-1,L)} (P^{(0)}, Q^{(0)}; P^{(0)}, Q^{(0)})
\]

\[
= \sum_{n_r = -\infty}^{\infty} \frac{1}{\mu_{n_r,\kappa} - 1} \int_0^\infty dr r^{-L-1} \left[ P^{(0)}(r) S^{(0)}_{n_r,\kappa}(r) + Q^{(0)}(r) T^{(0)}_{n_r,\kappa}(r) \right]
\]

\[
\times \int_0^\infty dr' r'^L \left[ \mu_{n_r,\kappa} P^{(0)}(r') S^{(0)}_{n_r,\kappa}(r') + Q^{(0)}(r') T^{(0)}_{n_r,\kappa}(r') \right] \quad (\kappa = L - L - 1).
\] (6.13)

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

\[
\int_0^\infty dr r^{-L-1} \left[ P^{(0)}(r) S^{(0)}_{n_r,\kappa}(r) + Q^{(0)}(r) T^{(0)}_{n_r,\kappa}(r) \right]
\]

\[
= -\left( \frac{2Z}{a_0} \right)^L \frac{\sqrt{\zeta(N_{n_r,\kappa} - \kappa)\gamma_1(N_{n_r,\kappa} + \kappa)} - (n_r + \gamma_\kappa - \gamma_1 + L)}{a_0 |n_r| \Gamma(N_{n_r,\kappa} - \kappa) \Gamma(2\gamma_1 + 1) \Gamma(|n_r| + 2\gamma_\kappa + 1)} \times \frac{\Gamma(\gamma_\kappa + \gamma_1 - L) \Gamma(|n_r| + 2\gamma_\kappa + L)}{\Gamma(\gamma_\kappa - 2\gamma_1 + L + 1)} \left( Z < \alpha^{-1} \frac{\sqrt{4L^2 - 1}}{2L} \text{ for } \kappa = L \right),
\] (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 \(\sigma_{EL \rightarrow EL,\kappa}\):

\[
\sigma_{EL \rightarrow EL,\kappa} = \frac{2|\kappa|}{Z(\kappa + 1)(2L + 1)^2}
\]

\[
\times \left\{ -1 + \frac{\gamma_1(\kappa + 1) - L][\gamma_1(\kappa + 1) + L + 1][\Gamma(\gamma_\kappa + \gamma_1 + L)]\Gamma(\gamma_\kappa + \gamma_1 + L + 1)}{\Gamma(\gamma_\kappa - 2\gamma_1 + 1) \Gamma(2\gamma_1 + 1) \Gamma(2\gamma_\kappa + 1) \Gamma(\gamma_\kappa + \gamma_1 + L)} \times 3F_2 \left\{ \gamma_\kappa - \gamma_1 + L + 1, \gamma_\kappa - \gamma_1 + L, \frac{\gamma_\kappa - \gamma_1 + 1}{\gamma_\kappa - \gamma_1 + 2, 2\gamma_\kappa + 1} \right. \right\} \quad (\kappa = L - L - 1).
\] (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), (4.11) 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 [11] Eq. (7.4.4.1)]

\[
\frac{\Gamma(b_2)\Gamma(s)}{\Gamma(b_2 - a_2)\Gamma(s + a_2)} 3F_2 \left\{ \begin{array}{c} b_1 - a_1, b_1 - a_3, a_2 \\ b_1, s + a_2 \end{array} \right\} ; 1 \right\}
\]

\[
|s = b_1 + b_2 - a_1 - a_2 - a_3; \text{Re } s > 0; \text{Re } (b_2 - a_2) > 0\],
\] (6.16)
and this casts Eq. (6.15) into

$$
\sigma_{\text{EL} \rightarrow \text{L}, \kappa} = \frac{2|\kappa|}{Z(\kappa + 1)(2L + 1)^2} \left\{ -1 + \frac{\gamma_1(\kappa + 1) - L}{(\gamma_\kappa - \gamma_1 + 1)(\gamma_\kappa + \gamma_1 - L)} \right. \\
\times F_2 \left( \begin{array}{c} -L + 1, 1, \gamma_\kappa - \gamma_1 - L  \\ \gamma_\kappa - \gamma_1 + 2, \gamma_\kappa + \gamma_1 - L + 1 \end{array} ; 1 \right) \right\} (\kappa = L, -L - 1). \tag{6.17}
$$

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

$$
\sigma_{\text{EL} \rightarrow \text{L}, L} = \frac{2L}{Z(L + 1)(2L + 1)^2} \left\{ -1 + \frac{L(\gamma_1 + 1)(\gamma_1 L + 1) - L}{(\gamma_\kappa - \gamma_1 + 1)(\gamma_\kappa + \gamma_1 - L)} \right. \\
\times F_2 \left( \begin{array}{c} -L + 1, 1, \gamma_\kappa - \gamma_1 - L  \\ \gamma_\kappa - \gamma_1 + 2, \gamma_\kappa + \gamma_1 - L + 1 \end{array} ; 1 \right) \right\}, \tag{6.18a}
$$

and

$$
\sigma_{\text{EL} \rightarrow \text{L}, -L - 1} = \frac{2(L + 1)}{Z(L + 1)(2L + 1)^2} \left\{ 1 - \frac{L(\gamma_1 + 1)(\gamma_1 L + 1) - L}{(\gamma_\kappa - \gamma_1 + 1)(\gamma_\kappa + \gamma_1 - L)} \right. \\
\times F_2 \left( \begin{array}{c} -L + 1, 1, \gamma_\kappa - \gamma_1 - L  \\ \gamma_\kappa - \gamma_1 + 2, \gamma_\kappa + \gamma_1 - L + 1 \end{array} ; 1 \right) \right\}, \tag{6.18b}
$$

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

$$
\sigma_{\text{EL} \rightarrow \text{L}} = \frac{2}{ZL(L + 1)(2L + 1)^2} \left\{ 1 + \frac{L^2(L + 1)(\gamma_1 + 1)\gamma_1 L + 1) - L}{(2L + 1)(\gamma_\kappa - \gamma_1 + 1)(\gamma_\kappa + \gamma_1 - L)} \right. \\
\times F_2 \left( \begin{array}{c} -L + 1, 1, \gamma_\kappa - \gamma_1 - L  \\ \gamma_\kappa - \gamma_1 + 2, \gamma_\kappa + \gamma_1 - L + 1 \end{array} ; 1 \right) \right\}. \tag{6.19}
$$

At the first sight, it might seem that the constraint on $Z$, under which the above formula is valid, is the one in Eq. (6.13). This is indeed the case if $L \geq 2$, but for $L = 1$ the situation is different. A closer look at the left-hand side of Eq. (6.14) and at Eq. (5.27) 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 $S_{n_\kappa}^{(0)}(r)$ and $T_{n_\kappa}^{(0)}(r)$. However, it is easy to show that the series

$$
\tilde{R}_1^{(-2,1)}(P^{(0)}, Q^{(0)}, P^{(0)}, Q^{(0)}) = \sum_{n_\kappa = -\infty}^{\infty} \frac{1}{\mu_{n_\kappa}^{(0)}} \left[ P^{(0)}(r)S_{n_\kappa}^{(0)}(r) + Q^{(0)}(r)T_{n_\kappa}^{(0)}(r) \right] \\
\times \int_0^\infty dr' r' \left[ \mu_{n_\kappa}^{(0)} P^{(0)}(r')S_{n_\kappa}^{(0)}(r') + Q^{(0)}(r')T_{n_\kappa}^{(0)}(r') \right], \tag{6.20a}
$$

where

$$
\tilde{S}_{n_\kappa}^{(0)}(r) = \sqrt{\frac{(1 + \gamma_1)(|n_\kappa| + 2\gamma_1)|n_\kappa|!}{2ZN_{n_\kappa}(N_{n_\kappa} - 1)I(|n_\kappa| + 2\gamma_1)}} \\
\times \left( \frac{2Zr}{a_0} \right)^{\gamma_1} e^{-Zr/a_0} \left[ |n_\kappa| - 1(0) + \frac{1 - N_{n_\kappa} - 1}{|n_\kappa| + 2\gamma_1} |n_\kappa| \right]. \tag{6.21a}
$$
and

\[ T_{n,L}(r) = \sqrt{\frac{(1 - \gamma_1)(|n_r| + 2\gamma_1)|n_r|!}{2ZN_{n,L}(N_{n,L} - 1)!|n_r| + 2\gamma_1}} \times \left( \frac{2Zr}{a_0} \right)^{\gamma_1} e^{-Zr/a_0} \left[ \frac{F(2\gamma_1)}{|n_r| - 1} - \frac{1 - N_{n,L}}{|n_r| + 2\gamma_1} L^{2\gamma_1}(0) \right], \]

(6.21b)
gives a null contribution to the integral \( R_4^{(-2,1)}(P^{(0)}, Q^{(0)}; P^{(0)}, Q^{(0)}) \). 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 \( \sigma_{EL \rightarrow EL} \) displayed in Eq. (6.19) is

\[ Z < \begin{cases} \alpha^{-1} & \text{for } L = 1 \\ \alpha^{-1} \frac{4L^2 - 1}{2L} & \text{for } L \geq 2. \end{cases} \]

(6.22)

As it holds that \( L \geq 1 \), 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 \( \sigma_{EL \rightarrow EL} \) with \( L \) constrained by \( 1 \leq L \leq 4 \) are displayed in Table IX.

[Place for Table IX]

Since only elementary functions are involved, numerical values of \( \sigma_{EL \rightarrow EL} \), 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 shall derive the quasi-relativistic representations for the shielding constants \( \sigma_{EL \rightarrow EL} \). Somewhat surprisingly, this appears to be a bit more involved than in the case of the three far-field susceptibilities analyzed in Secs. 3 to 5. Referring to Eqs. (3.43) and (3.44), the quasi-relativistic approximations for the two \( 3F_2(1) \) functions in Eqs. (6.18a) and (6.18b) are found to be

\[ 3F_2 \left( \begin{array}{c} -L + 1, 1 \\ \gamma_L - \gamma_1 + L \end{array} \right) \left( \begin{array}{c} L - 1 \\ 2L(L + 1) \end{array} \right) \approx \left( \frac{3L + 1}{4L(L + 1)} \right) - (\alpha Z)^2 \frac{L - 1}{4L(L + 1)} \frac{L^2 - 5}{3(L + 2)} 3F_2 \left( \begin{array}{c} -L + 3, 1, 1 \\ L + 1, L + 3, 4 \end{array} \right); \]

(6.23)

and

\[ 3F_2 \left( \begin{array}{c} -L + 1, 1, \gamma_L + 1 - \gamma_1 - L \\ \gamma_L + 1 - \gamma_1 \end{array} \right) \left( \begin{array}{c} L(L - 1) \\ 6(L + 1)(L + 2) \end{array} \right) 3F_2 \left( \begin{array}{c} -L + 2, 1, 1 \\ L + 3, 4 \end{array} \right); \]

(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. (6.10), we obtain

\[ 3F_2 \left( \begin{array}{c} -L + 2, 1, 1 \\ L + 3, 4 \end{array} \right) = -\frac{3(L + 2)(5L + 4)}{2L(L + 1)} + \frac{6(L + 2)(L + 1)}{L(L - 1)} [\psi(2L + 1) - \psi(L + 2)] \]

(6.25)

and

\[ 3F_2 \left( \begin{array}{c} -L + 3, 1, 1 \\ L + 3, 4 \end{array} \right) = -\frac{3(L + 2)(5L + 1)}{2L(L - 1)} + \frac{6(L + 2)(L + 1)}{(L - 1)(L - 2)} [\psi(2L) - \psi(L + 2)] \]

(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’s rule), which allows us to rewrite Eqs. (6.23) and (6.24) as

\[
3F_2\left(\begin{array}{c}
-L + 1, 1, \gamma_L - \gamma_1 - L \\
\gamma_L - \gamma_1 - 1, \gamma_L + \gamma_1 - L + 1
\end{array}\right)
\cong \frac{3L + 1}{2(L + 1)} - (\alpha Z)^2 \frac{(L - 1)(2L + 1)}{2L(L + 1)} \left[ \psi(2L + 1) - \psi(L + 1) - \frac{L + 1}{2L + 1} \right]
\] (6.27)

and

\[
3F_2\left(\begin{array}{c}
-L + 1, 1, \gamma_{L+1} - \gamma_1 - L \\
\gamma_{L+1} - \gamma_1 - 1, \gamma_{L+1} + \gamma_1 - L + 1
\end{array}\right)
\cong 1 - (\alpha Z)^2 \frac{2L + 1}{L + 1} \left[ \psi(2L + 1) - \psi(L + 1) - \frac{L(5L + 7)}{4(L + 1)(2L + 1)} \right].
\] (6.28)

respectively. Inserting the above two estimates into Eqs. (6.18a) and (6.18b) and passing to the quasi-relativistic limit with the factors multiplying the two \(3F_2\)'s, one arrives at

\[
\sigma_{E \rightarrow E L} \cong \frac{2}{Z(L + 1)(2L + 1)} \left\{ 1 - (\alpha Z)^2 \frac{L}{L + 1} \left[ \psi(2L + 1) - \psi(L + 1) + \frac{6L^4 + L^3 + L^2 - 2L - 2}{4L(L - 1)(2L + 1)} \right] \right\}
\] (6.29a)

and

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

Hence, we infer the following formula for the quasi-relativistic approximations of the electric multipole shielding constants:

\[
\sigma_{E \rightarrow E L} \cong \frac{2}{ZL(L + 1)} \left\{ 1 - (\alpha Z)^2 \frac{2L - 1}{2L + 1} \left[ \psi(2L + 1) - \psi(L + 1) - \frac{L^3 - 2L^2 + L - 1}{2L(2L - 1)} \right] \right\}.
\] (6.30)

Estimates of \(\sigma_{E \rightarrow E L}\) resulting from Eq. (6.30) are presented in Table X for \(1 \leq L \leq 4\).

We have verified numerically that the quasi-relativistic 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 \((2L - 2)!\) by \((2L - n)!\). In addition, we remark that the quasi-relativistic approximations to \(\sigma_{E \rightarrow E L}\) 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.

7 Near-nucleus magnetic multipole moments of the atom in the multipole electric field and near-nucleus \(E_{L \rightarrow M(L + 1)}\) multipole cross-susceptibilities

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

Next, we shall consider the near-nucleus magnetic multipole moments of the atom in the \(2^L\)-pole electric field. In agreement with Eq. (13.38), the spherical components of the \(2^L\)-pole moment of
that sort are given by

\[ N_{\lambda\mu} = i \sqrt{\frac{4\pi(\lambda + 1)}{\lambda(2\lambda + 1)}} \int_{\mathbb{R}^3} d^3r \, r^{-\lambda-1} Y_{\lambda\mu}(n_r) \cdot \mathbf{j}(r), \]  

(7.1)

where \( \mathbf{j}(r) \) 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

\[ N_{\lambda\mu} = -i \sqrt{\frac{4\pi}{2\lambda + 1}} \int_{\mathbb{R}^3} d^3r \, r^{-\lambda-1} Y_{\lambda\mu}(n_r) \Lambda \cdot \mathbf{j}(r). \]  

(7.2)

Approximating the current as in Eq. (4.6), yields

\[ N_{\lambda\mu} \simeq N_{\lambda\mu}^{(0)} + N_{\lambda\mu}^{(1)}, \]  

(7.3)

with

\[ N_{\lambda\mu}^{(0)} = -i \sqrt{\frac{4\pi}{2\lambda + 1}} \int_{\mathbb{R}^3} d^3r \, r^{-\lambda-1} Y_{\lambda\mu}(n_r) \Lambda \cdot \mathbf{j}^{(0)}(r). \]  

(7.4)

and

\[ N_{\lambda\mu}^{(1)} = -i \sqrt{\frac{4\pi}{2\lambda + 1}} \int_{\mathbb{R}^3} d^3r \, r^{-\lambda-1} Y_{\lambda\mu}(n_r) \Lambda \cdot \mathbf{j}^{(1)}(r). \]  

(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 those in Eqs. (4.10) and (4.11), respectively. This immediately allows us to write

\[ N_{\lambda} \simeq N_{\lambda}^{(0)} \delta_{\lambda 1} + N_{\lambda}^{(0)} (\delta_{\lambda, L-1} + \delta_{\lambda, L+1}), \]  

(7.6)

where

\[ N_{1}^{(0)} = -\frac{4}{3} \varepsilon \nu \int_{0}^{\infty} dr \, r^{-2} P^{(0)}(r) Q^{(0)}(r) \]  

(7.7)

and

\[ N_{\lambda}^{(1)} = (4\pi\varepsilon_0)c \frac{2\sqrt{2}(\lambda + 1)}{(2\lambda + 1)\sqrt{(2L + 1)(\Lambda + 1)}} R_{\kappa\lambda}^{(-\lambda-1,L)}(Q^{(0)}, P^{(0)}, P^{(0)}, Q^{(0)}) \{ \nu \otimes \mathbf{C}_{L}^{(1)} \}_{\lambda} \]  

(\( \lambda = L \mp 1, \lambda \neq 0 \)),  

(7.8)

with \( \kappa_{\lambda} \) 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. (5.12)].

Straightforward evaluation of the radial integral in Eq. (7.7) gives the following closed-form representation of the permanent dipole moment \( N_{1}^{(0)} \):

\[ N_{1}^{(0)} = \frac{8}{3\gamma_1(2\gamma_1 - 1)} \frac{\mu_B Z^3}{\alpha_0^3} \nu \left( Z < \alpha^{-1}\frac{\sqrt{2}}{2} \right), \]  

(7.9)

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

### 7.2 Atomic near-nucleus multipole EL → M(L ± 1) cross-susceptibilities

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

\[ N_{\lambda}^{(1)} = (4\pi\varepsilon_0)c \sigma_{EL \rightarrow M\Lambda} \left\{ \nu \otimes \mathbf{C}_{L}^{(1)} \right\}_{\lambda} \]  

(\( \lambda = L \mp 1, \lambda \neq 0 \)),  

(7.10)
where $N_{(1)}^{(1)}$ has been given in Eq. (7.3). Recalling the expression (4.36) for the Clebsch–Gordan coefficient $(10L0|00)$ with $\lambda = L \mp 1$, yields the susceptibility $\sigma_{EL \rightarrow MA}$ in the form

$$\sigma_{EL \rightarrow MA} = \frac{2(\lambda + 1)(\lambda - L)}{(2\lambda + 1)(2L + 1)} \rho_{\kappa_{\lambda}}^{(-\lambda - 1, L)}(Q^{(0)}, P^{(0)}, P^{(0)}, Q^{(0)}) \quad (\lambda = L \mp 1; \lambda \neq 0). \quad (7.11)$$

In view of Eqs. (3.14) and (3.26), we may write

$$\rho_{\kappa_{\lambda}}^{(-\lambda - 1, L)}(Q^{(0)}, P^{(0)}, P^{(0)}, Q^{(0)})$$

$$= \sum_{n_r} \frac{1}{P_{n_r, \kappa_{\lambda}}} \int_0^\infty dr \frac{1}{r^{\lambda - 1}} \left[ Q^{(0)}(r)S_{n_r, \kappa_{\lambda}}^{(0)}(r) + P^{(0)}(r)T_{n_r, \kappa_{\lambda}}^{(0)}(r) \right]$$

$$\times \int_0^\infty dr' \rho_{\kappa_{\lambda}}^{(0)}(r'P_{n_r, \kappa_{\lambda}}^{(0)}(r') + Q^{(0)}(r')T_{n_r, \kappa_{\lambda}}^{(0)}(r'))$$

$$\quad (\lambda = L \mp 1; \lambda \neq 0). \quad (7.12)$$

The second of the two integrals on the right-hand side of Eq. (7.12) is the same which has appeared in the last four sections, and its value has been given in Eq. (3.51). As regards the first one, its value may be deduced from Eq. (4.39), after the replacement $\lambda \rightarrow -\lambda - 1$ is made in the latter, and this gives

$$\int_0^\infty dr \frac{1}{r^{\lambda - 1}} \left[ Q^{(0)}(r)S_{n_r, \kappa_{\lambda}}^{(0)}(r) + P^{(0)}(r)T_{n_r, \kappa_{\lambda}}^{(0)}(r) \right]$$

$$= - \alpha Z (\frac{2Z}{a_0})^\lambda \sqrt{2} \sqrt{N_{n_r, \kappa_{\lambda}} - \kappa_{\lambda}}$$

$$\times \frac{\Gamma(\gamma_{\kappa_{\lambda}} + \gamma - \lambda)\Gamma(n_r + \gamma_{\kappa_{\lambda}} - \gamma + 1 + \lambda + 1)}{\Gamma(\gamma_{\kappa_{\lambda}} - \gamma + 1 + \lambda + 1)}$$

$$\left( Z < \alpha^{-1} \frac{\sqrt{2L + 1)(2L + 3)}{2L + 1} \right) \quad \text{for } \lambda = L + 1), \quad (7.13)$$

where the constraint, henceforth tacitly assumed to hold, guarantees the integral in question converges at its lower limit. Plugging Eqs. (6.32) and (7.13) into Eq. (7.12), and then the latter into Eq. (7.11), after transformations which are already routine at this stage, we obtain

$$\sigma_{EL \rightarrow MA} = \frac{\alpha a_0 L - \lambda}{Z L - \lambda} \frac{(\lambda + 1)(\lambda - L)\Gamma(2\gamma_{\kappa_{\lambda}} - \lambda + L + 1)}{2L - \lambda(\kappa_{\lambda} + 1)(2\lambda + 1)(2L + 1)\Gamma(2\gamma_{\kappa_{\lambda}} + 1)}$$

$$\times \left\{ 1 + \frac{\lambda[\gamma_{\kappa_{\lambda}} + 1 + L + 1]\Gamma(\gamma_{\kappa_{\lambda}} + \gamma - 1 + 1)\Gamma(\gamma_{\kappa_{\lambda}} - \gamma + 1 + 1)}{(\gamma_{\kappa_{\lambda}} - \gamma + 1 + 1)\Gamma(2\gamma_{\kappa_{\lambda}} - \lambda + L + 1)\Gamma(2\gamma_{\kappa_{\lambda}} + 1)} \right\}$$

$$\times \frac{\gamma_{\kappa_{\lambda}} - \gamma + 1 + 1, \gamma_{\kappa_{\lambda}} - \gamma - L, \gamma_{\kappa_{\lambda}} - \gamma + 1,}{\gamma_{\kappa_{\lambda}} - \gamma + 2, 2\gamma_{\kappa_{\lambda}} + 1} \right\}$$

\begin{equation}
\begin{aligned}
\quad (\lambda = L \mp 1; \lambda \neq 0).
\end{aligned}
\end{equation}

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

$$\sigma_{EL \rightarrow MA} = \frac{\alpha a_0 L - \lambda}{Z L - \lambda} \frac{(\lambda + 1)(\lambda - L)\Gamma(2\gamma_{\kappa_{\lambda}} - \lambda + L + 1)}{2L - \lambda(\kappa_{\lambda} + 1)(2\lambda + 1)(2L + 1)\Gamma(2\gamma_{\kappa_{\lambda}} + 1)}$$

$$\times \left\{ 1 + \frac{\lambda[\gamma_{\kappa_{\lambda}} + 1 + L + 1]}{(\gamma_{\kappa_{\lambda}} - \gamma + 1 + 1)\Gamma(2\gamma_{\kappa_{\lambda}} + 1)} \right\}$$

$$\times \left\{ -\lambda + 1 + 1, \gamma_{\kappa_{\lambda}} - \gamma - L, \gamma_{\kappa_{\lambda}} + \gamma - \lambda + 1 + 1 \right\}$$

\begin{equation}
\begin{aligned}
\quad (\lambda = L \mp 1; \lambda \neq 0).
\end{aligned}
\end{equation}
where the \( _3F_2(1) \) function is a truncating one. Hence, we find that the explicit representations of the two cross-susceptibilities \( \sigma_{EL \to M(L^3)} \) are

\[
\sigma_{EL \to M(L-1)} = -\frac{\alpha_0}{Z} \frac{L(2\gamma_1 + 1)}{(L + 1)^2(4L^2 - 1)} \left\{ 1 + \frac{(L^2 - 1)(\gamma_1 + 1)}{(\gamma_L - \gamma_1 + 1)(\gamma_L + \gamma_1 - L + 1)} \right\} \times _3F_2 \left( \begin{array}{c} -L + 2, 1, \gamma_L - \gamma_1 - L \\ \gamma_L - \gamma_1 + 2, \gamma_L + \gamma_1 - L + 2 ; 1 \end{array} \right) \quad (L \neq 1) \tag{7.16}
\]

and

\[
\sigma_{EL \to M(L+1)} = -\frac{\alpha Z}{\alpha_0 \gamma_L L(2L + 1)(2L + 3)} \left\{ 1 - \frac{(L + 1)(\gamma_1 - L - 1)}{(\gamma_{L+1} - \gamma_1 + 1)(\gamma_{L+1} + \gamma_1 - L - 1)} \right\} \times _3F_2 \left( \begin{array}{c} -L, 1, \gamma_{L+1} - \gamma_1 - L \\ \gamma_{L+1} - \gamma_1 + 2, \gamma_{L+1} + \gamma_1 - L - 1 ; 1 \end{array} \right) \left( Z < \alpha^{-1} \sqrt{\frac{(2L + 1)(2L + 3)}{2L + 1}} \right). \tag{7.17}
\]

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

[Place for Table XI]

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

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

and

\[
_3F_2 \left( \begin{array}{c} -L, 1, \gamma_{L+1} - \gamma_1 - L \\ \gamma_{L+1} - \gamma_1 + 2, \gamma_{L+1} + \gamma_1 - L - 1 ; 1 \end{array} \right) \approx 1 - (\alpha Z)^2 \frac{L^2}{4(L + 1)(L + 2)} _3F_2 \left( \begin{array}{c} -L + 1, 1, 1 \\ L + 3, 3 ; 1 \end{array} \right), \tag{7.19}
\]

which, with the aid of the identities

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

[cf. Eq. (E.11)] and

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

[cf. Eq. (E.3)], may be rewritten as

\[
_3F_2 \left( \begin{array}{c} -L + 2, 1, \gamma_L - \gamma_1 - L \\ \gamma_L - \gamma_1 + 2, \gamma_L + \gamma_1 - L + 2 ; 1 \end{array} \right) \approx \frac{4L + 1}{3(L + 1)} - (\alpha Z)^2 \frac{4L^2 - 1}{3(L + 1)} \left[ \psi(2L + 1) - \psi(L + 1) \right] - \frac{7(L + 1)(4L - 3)}{12(4L^2 - 1)} \tag{7.22}
\]
and
\[
3F2 \left( \begin{array}{c}
-L, 1, \gamma L+1 - \gamma_1 - L \\
\gamma L+1 - \gamma_1 + 1, \gamma L+1 + \gamma_1 - L, 1
\end{array} ; 1 \right) \simeq 1 - (\alpha Z)^2 \frac{L}{L+1} \left[ \psi(2L+2) - \psi(L+2) - \frac{L}{2(L+1)} \right],
\]
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 quasi-relativistic approximations
\[
\sigma_{EL\rightarrow M(L-1)} \simeq -\frac{\alpha a_0}{Z} \frac{1}{L+1} \left( 1 - (\alpha Z)^2 \frac{L-1}{L} \left[ \psi(2L) - \psi(L) - \frac{L(4L^2 - 3L - 5)}{4(L-1)(4L^2 - 1)} \right] \right) \quad (L \neq 1)
\]
and
\[
\sigma_{EL\rightarrow M(L+1)} \simeq -\frac{\alpha Z}{a_0} \frac{4(L+2)}{L(2L+1)(2L+3)} \times \left\{ 1 - (\alpha Z)^2 \frac{L}{2(L+1)} \left[ \psi(2L+2) - \psi(L+1) - \frac{(L+1)(L+4)}{2L} \right] \right\}
\]
Particular cases of the later two formulas are displayed in Table XII.

8 Near-nucleus magnetic toroidal multipole moments of the atom in the multipole electric field and near-nucleus $EL \rightarrow TL$ multipole cross-susceptibilities

8.1 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 $U^\lambda$. According to Eq. (8.1), their spherical components may be defined as
\[
U_{\lambda \mu} = -\frac{1}{\lambda} \sqrt{\frac{4\pi}{2\lambda + 1}} \int_{\mathbb{R}^3} d^3r \ r^{-\lambda-1} Y_{\lambda \mu}(n_r) r \cdot j(r).
\]
In the weak-perturbing-field regime, which we consider in this paper, after exploiting Eq. (4.6), we have
\[
U_{\lambda \mu} \simeq U_{\lambda \mu}^{(0)} + U_{\lambda \mu}^{(1)},
\]
with
\[
U_{\lambda \mu}^{(0)} = -\frac{1}{\lambda} \sqrt{\frac{4\pi}{2\lambda + 1}} \int_{\mathbb{R}^3} d^3r \ r^{-\lambda-1} Y_{\lambda \mu}(n_r) r \cdot j^{(0)}(r)
\]
and
\[
U_{\lambda \mu}^{(1)} = -\frac{1}{\lambda} \sqrt{\frac{4\pi}{2\lambda + 1}} \int_{\mathbb{R}^3} d^3r \ r^{-\lambda-1} Y_{\lambda \mu}(n_r) r \cdot j^{(1)}(r)
\]
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. 5 one may show that the isolated atom in the ground state does not possess any non vanishing moments of the sort considered,
\[
U_{\lambda}^{(0)} = 0,
\]
and that the only induced moment is the one with the multipolar symmetry identical to that of the perturbing electric field, i.e.,
\[
U_{\lambda} \simeq U_{\lambda}^{(1)} \delta_{\lambda L},
\]
we arrive at

$$U^{(1)}_L = (4\pi e_0)c \frac{2i}{(2L+1)^2} \sqrt{\frac{L+1}{L}} \times \left[ R^{(-L,L)}_L (Q^{(0)}, -P^{(0)}; P^{(0)}, Q^{(0)}) - R^{(-L,L)}_{-L-1} (Q^{(0)}, -P^{(0)}; P^{(0)}, Q^{(0)}) \right] \{ \nu \otimes C^{(1)}_L \}_L$$

(8.7)

[for the definition of the double radial integrals $R^{(-L,L)}_L (Q^{(0)}, -P^{(0)}; P^{(0)}, Q^{(0)})$, see Eq. (3.13)].

8.2 Atomic near-nucleus multipole $EL \to TL$ cross-susceptibilities

In complete analogy to the far-field case discussed in Sec. 5.2, we define the near-nucleus multipole $EL \to TL$ cross-susceptibilities through the relation

$$\sigma_{EL \to TL} = \sigma_{EL \to TL,L} + \sigma_{EL \to TL,-L-1},$$

(8.9)

where

$$\sigma_{EL \to TL,L} = \frac{2 \text{sgn}(\kappa)}{L(2L+1)^2} R^{(-L,L)}_L (Q^{(0)}, -P^{(0)}; P^{(0)}, Q^{(0)}) \quad (\kappa = L, -L - 1).$$

(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

$$R^{(-L,L)}_L (Q^{(0)}, -P^{(0)}; P^{(0)}, Q^{(0)}) = \sum_{\nu=-\infty}^{\infty} \rho^{(0)}_{\nu_L,-\nu}\int_0^\infty \int_0^\infty \rho^L_r r^{-L} \left[ Q^{(0)}(r) S^{(0)}_{\nu_L,-\nu}(r) - P^{(0)}(r) T^{(0)}_{\nu_L,-\nu}(r) \right]$$

$$\times \int_0^\infty \int_0^\infty \rho^L_{r'} r'^{-L} \left[ S^{(0)}_{\nu_L,-\nu}(r') + Q^{(0)}(r') T^{(0)}_{\nu_L,-\nu}(r') \right] dr r^{-L} dr' r'^{-L}.$$ (8.11)

With no difficulty, from Eqs. (2.11), (5.27) and (3.31) one finds that

$$\int_0^\infty \int_0^\infty \rho^L_r r^{-L} \left[ Q^{(0)}(r) S^{(0)}_{\nu_L,-\nu}(r) - P^{(0)}(r) T^{(0)}_{\nu_L,-\nu}(r) \right]$$

$$= \alpha Z \left( \frac{2Z}{\alpha_0} \right)^{L-1} \frac{L(2L+1)^2}{\sqrt{2|\nu_L|(|\nu_L| + 2\gamma)}},$$

$$\times \Gamma(\gamma_L + \gamma_L - L + 1) \Gamma(\gamma) \Gamma(\gamma_L + 1) \Gamma(\gamma_L + 2\gamma + 1).$$

(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 $\sum_{\nu_L=-\infty}^{\infty} (\cdots)$ into the one of the form $\sum_{\nu_L=0}^{\infty} (\cdots)$, we arrive at

$$\sigma_{EL \to TL,L} = -\frac{\alpha_0 \text{sgn}(\kappa) \gamma \gamma + \gamma_L + L + 1)}{L(2L+1)^2(\gamma_L + \gamma_L - L + 1) \Gamma(\gamma_L + \gamma_L + L + 1)} \times \frac{\alpha Z}{\sqrt{2|\nu_L|(|\nu_L| + 2\gamma)}}$$

$$\times \frac{\gamma_L - \gamma_L + L}{\gamma_L - \gamma_L - L + 1} \frac{\gamma_L + \gamma_L + L + 1}{\gamma_L - \gamma_L + 2, 2\gamma_L + 1}.$$ (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

\[
\sigma_{E\ell\rightarrow TL, \kappa} = -\frac{a_0}{Z} \frac{\text{sgn}(\kappa)(2\gamma + 1)[\gamma + 1 + L + 1]}{L(2L + 1)^2(\gamma + 1)(\gamma + L + 1)} \times _3F_2\left( -L + 2, 1, \gamma + L + 1 + 1 : 1 \right) \quad (\kappa = L, -L - 1). \tag{8.14}
\]

Hence, the cross-susceptibility \( \sigma_{E\ell\rightarrow TL} \) is the sum of

\[
\sigma_{E\ell\rightarrow TL, L} = -\frac{a_0}{Z} \frac{(L + 1)(\gamma + 1)(2\gamma + 1)}{L(2L + 1)^2(\gamma + 1)(\gamma + L + 1)} \times _3F_2\left( \gamma + L - 1, \gamma + L - L, \gamma + L + 1 + 1 : 1 \right)
\]

and

\[
\sigma_{E\ell\rightarrow TL, -L - 1} = -\frac{a_0}{Z} \frac{(2\gamma + 1)(L + L - 1)}{L(2L + 1)^2(\gamma + 1)(\gamma + L + 1)} \times _3F_2\left( \gamma + L + 1 + 1, \gamma + L + L, \gamma + L + 1 + 1 : 1 \right), \tag{8.15a}
\]

and is explicitly given by

\[
\sigma_{E\ell\rightarrow TL} = -\frac{a_0}{Z} \frac{(L + 1)(\gamma + 1)}{L(2L + 1)^2} \left\{ \frac{\gamma + 1}{(\gamma + L - 1)(\gamma + L + 1)} \times _3F_2\left( \gamma + L - 1, \gamma + L - L, \gamma + L + 1 + 1 : 1 \right) + \frac{1}{(L + 1)(\gamma + L - 1)(\gamma + L + 1)} \times _3F_2\left( \gamma + L + 1 + 1, \gamma + L + L, \gamma + L + 1 + 1 : 1 \right) \right\}. \tag{8.16}
\]

For \( L \geq 2 \), both hypergeometric series on the right-hand side of Eq. (8.10) truncate, and consequently the corresponding cross-susceptibilities \( \sigma_{E\ell\rightarrow TL} \) 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 \( \sigma_{E\ell\rightarrow TL} \) with \( 1 \leq L \leq 4 \) are presented in Table XIII. In turn, in Table XIV we provide numerical data for the dipole cross-susceptibility \( \sigma_{E1\rightarrow T1} \) for selected values of the nuclear charge number \( Z \).

[Place for Tables XIII and XIV]

We move to the derivation of the quasi-relativistic 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. 7.2, and the approximation to it is given in Eq. (8.22). In turn, for the hypergeometric function in Eq. (8.15b) we have

\[
_3F_2\left( -L + 2, 1, \gamma_L + 1 - \gamma - L \gamma_L + 1 + \gamma_L + 1 + \gamma - L + 2 ; 1 \right) \simeq 1 - (\alpha Z)^2 \frac{L(L - 2)}{8(L + 1)(L + 2)} _3F_2\left( -L + 3, 1, 1 L + 3, 5 ; 1 \right). \tag{8.17}
\]

From Eq. (8.11) we have

\[
_3F_2\left( -L + 3, 1, 1 L + 3, 5 ; 1 \right) = \frac{16(L + 2)(2L + 1)}{(L - 1)(L - 2)}[\psi(2L) - \psi(L + 2)] - \frac{4(L + 2)(16L^2 + 17L + 3)}{3L(L^2 - 1)} \tag{8.18}
\]
The explicit forms of the quasi-relativistic approximations to \( \sigma_3 \) procedure) and consequently the expression on the right-hand side are only apparent and are removable via the passage to the limit procedure. Using Eqs. (7.22) and (8.19), after some algebraic simplifications we obtain

\[
\sigma_{E \rightarrow TL, L} \simeq -\frac{\alpha a_0}{Z} \frac{4L+1}{L^2(2L+1)^2} \times \left\{ 1 - (\alpha Z)^2 \frac{2L(2L+1)}{L^2} \left[ \psi(2L+1) - \psi(L+1) - \frac{16L^2 + 21L - 1}{12(L+1)(2L+1)} \right] \right\}
\]

and

\[
\sigma_{E \rightarrow TL, L-1} \simeq -\frac{\alpha a_0}{Z} \frac{1}{L(L+1)(2L+1)^2} \times \left\{ 1 - (\alpha Z)^2 \frac{2L(2L+1)}{L^2} \left[ \psi(2L+1) - \psi(L+1) - \frac{L(L+3)}{4(2L+1)} \right] \right\}
\]

Hence, the sought approximate expression for the cross-susceptibility \( \sigma_{E \rightarrow TL} \) is

\[
\sigma_{E \rightarrow TL} \simeq -\frac{\alpha a_0}{Z} \frac{1}{L^2(L+1)} \left\{ 1 - (\alpha Z)^2 \frac{2L^4 - L^3 - 3L^2 - L + 1}{L(2L+1)(L^2 - 1)} \right\}
\]

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

\[
\psi'(1) = \frac{\pi^2}{6}, \quad \psi'(2) = \frac{\pi^2}{6} - 1
\]

are exploited, Eq. (8.21) becomes

\[
\sigma_{E \rightarrow T1} \simeq -\frac{\alpha a_0}{Z} \frac{1}{2} \left[ 1 - \left( \frac{3}{4} - \frac{\pi^2}{18} \right)(\alpha Z)^2 \right].
\]

The explicit forms of the quasi-relativistic approximations to \( \sigma_{E \rightarrow TL} \) for \( 1 \leq L \leq 4 \), resulting from Eqs. (8.22) and (8.21), are displayed in Table XV

9 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\( \mu \)-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. 3–8 with the aid of the Sturmian expansion of the Dirac–Coulomb Green function, are collected in Tables XVIII and XIX

[Place for Table XV]

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Because of space limitations, in Tables II, IV, V and VII embedded in Secs. 3–5, we have provided numerical values of the far-field susceptibilities $\alpha_L (\equiv \alpha_{EL \rightarrow EL})$, $\alpha_{EL \rightarrow M (L \pm 1)}$ and $\alpha_{EL \rightarrow TL}$, all with $1 \leq L \leq 4$, only for selected values of the nuclear charge number $Z$. A complete tabulation of values of these susceptibilities for all integer values of $Z$ from the range $1 \leq Z \leq 137$ will be presented elsewhere.

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, both for electric and magnetic perturbing fields, for the atom in energetically excited states belonging to the principal 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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**A Multi-pole 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 $\alpha_L$ and the second-order correction to atomic energy due to a perturbing static electric $2^L$-pole field defined in Sec. 2. 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. 2, the perturbed wave function of the atom may be approximated by

$$\Psi(r) \simeq \Psi^{(0)}(r) + \Psi^{(1)}(r) + \Psi^{(2)}(r). \quad (A.1)$$

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 $a_{\pm \frac{1}{2}}$ in Eq. (2.9) undetermined. Similarly, for the atomic energy in the field we may write

$$E \simeq E^{(0)} + E^{(1)} + E^{(2)} \quad (A.2)$$

with $E^{(0)}$ and $E^{(1)}$ given by Eqs. (2.16) and (2.27), respectively. Proceeding in the standard manner, from Eqs. (2.14), (A.1) and (A.2) we deduce that the corrections $\Psi^{(2)}(r)$ and $E^{(2)}$ solve

$$\left[-i\hbar \alpha \cdot \nabla + \beta mc^2 - \frac{Ze^2}{(4\pi\epsilon_0)r} - E^{(0)} \right] \Psi^{(2)}(r) = -[V_L^{(1)}(r) - E^{(1)}] \Psi^{(1)}(r) + E^{(2)} \Psi^{(0)}(r), \quad (A.3)$$

subject to the orthogonality constraints

$$\int_{\mathbb{R}^3} d^3r \, \Psi^{(0)\dagger}_m(r) \Psi^{(2)}(r) = 0 \quad (m = \pm \frac{1}{2}). \quad (A.4)$$

Projecting Eq. (A.3) from the left onto the unperturbed basis functions $\Psi^{(0)\dagger}_m(r)$ and then making use of Eqs. (2.9), (2.12), (2.16), (2.27) and (2.28), we arrive at the homogeneous algebraic system

$$\sum_{m' = -1/2}^{1/2} \left[V_L^{(1),m'} - E^{(2)} \delta_{mm'} \right] a_{m'} = 0 \quad (m = \pm \frac{1}{2}), \quad (A.5)$$
in which
\[ V_{L,m} = -\int_{\mathbb{R}^3} d^3r \int_{\mathbb{R}^3} d^3r' \Psi_m^+(r)V_L(r)\hat{G}(r,r')V_L^+(r')\Psi_m(r'). \] (A.6)

To simplify the expression on the right-hand side of Eq. (A.6), we make use of Eqs. (2.23), (2.10), (3.13) and (2.20), and also of the definitions (3.16) and (3.15). This yields
\[ V_{L,m}^{(1,1)} = -\left(4\pi\epsilon_0\right)\frac{4\pi}{2L + 1}\sum_{\kappa = -\infty}^{\infty} R_{\kappa}(L,L)(P^{(0)},Q^{(0)};P^{(0)},Q^{(0)}) \sum_{M = -L}^{L} \sum_{M' = -L}^{L} C_{LM}^{(1)} C_{LM'}^{(1)*} \]
\times \sum_{m_{\kappa} = -|\kappa|+1/2}^{1/2} \langle \Omega - 1m \Omega_{L,m_{\kappa}} | \Omega_{m_{\kappa}} \rangle Y_{L,m} \Omega_{L'-1m'}. \] (A.7)

Evaluation of the angular integrals with the help of Eq. (2.22) casts Eq. (A.7) into
\[ V_{L,m}^{(1,1)} = -\left(4\pi\epsilon_0\right)\sum_{\kappa = -\infty}^{\infty} \frac{\delta_{\kappa L} + \delta_{\kappa - L - 1}}{2L + 1} R_{\kappa}(L,L)(P^{(0)},Q^{(0)};P^{(0)},Q^{(0)}) \]
\times \left[ \delta_{m,1/2} \delta_{m',-1/2} \sum_{M = -L}^{L} (-)^M \frac{\kappa + M}{2K + 1} C_{LM}^{(1)*} C_{LM'}^{(1)*} \right.
\left. + \frac{\operatorname{sgn}(\kappa)\delta_{m,1/2} \delta_{m',-1/2}}{2K + 1} \sum_{M = -L}^{L} (-)^M \frac{\kappa - M}{2K + 1} C_{LM}^{(1)*} C_{LM'}^{(1)*} \right] \] (A.8)

The four sums over \( M \) may be simplified after evident symmetry properties of their summands are taken into account. One finds that
\[ \sum_{M = -L}^{L} (-)^M \frac{\kappa + M}{2K + 1} C_{LM}^{(1)*} C_{LM'}^{(1)*} = \frac{|\kappa|}{2L + 1} \sum_{M = -L}^{L} C_{LM}^{(1)*} C_{LM'}^{(1)} \] (\( \kappa = L, -L - 1 \)) (A.9)
and
\[ \sum_{M = -L}^{L} (-)^M \frac{(\kappa + M)(\kappa + M + 1)}{2K + 1} C_{LM}^{(1)*} C_{LM'}^{(1)*} = 0 \] (\( \kappa = L, -L - 1 \)). (A.10)

Hence, we deduce that
\[ V_{L,m}^{(1,1)} = -\delta_{mm'}(4\pi\epsilon_0)\left[ \frac{L}{(2L + 1)^2} R_{L}(L,L)(P^{(0)},Q^{(0)};P^{(0)},Q^{(0)}) \right. \]
\left. + \frac{L + 1}{(2L + 1)^2} R_{L-1}(L,L)(P^{(0)},Q^{(0)};P^{(0)},Q^{(0)}) \right] \sum_{M = -L}^{L} C_{LM}^{(1)*} C_{LM'}^{(1)*}. \] (A.11)

The matrix formed by the elements \( V_{L,m}^{(1,1)} \) is thus seen to be a multiple of the unit \( 2 \times 2 \) matrix. Recalling Eqs. (3.21) and (3.22), 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
\[ E^{(2)} = -\frac{1}{2}(4\pi\epsilon_0)\alpha_L C_L^{(1)*} C_L^{(1)} \] (A.12)

This result is very well known in the dipole \( (L = 1) \) case.
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 [39], which we wholeheartedly recommend to all readers interested in the subject.

B.1 General considerations

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

\[
A(r) = \frac{\mu_0}{4\pi} \int_{\mathbb{R}^3} d^3r' \frac{j(r')}{|r - r'|}.
\]  

(B.1)

Exploiting the multipole expansion

\[
\frac{1}{|r - r'|} = \sum_{L=0}^{\infty} \sum_{M=-L}^{L} \frac{4\pi}{2L + 1} \frac{r^L}{r^{L+1}} Y_{LM}^*(n_r) Y_{LM}(n'_r),
\]  

(B.2)

one finds that in the far-field \( (r \to \infty) \) and near-field \( (r \to 0) \) regions the vector potential \( A(r) \) behaves as

\[
A(r) \xrightarrow{r \to \infty} \sum_{L=0}^{\infty} A^{LL}(r)
\]  

(B.3)

and

\[
A(r) \xrightarrow{r \to 0} \sum_{L=0}^{\infty} A^{L,-L-1}(r),
\]  

(B.4)

respectively, where

\[
A^{L\lambda}(r) = \frac{\mu_0}{4\pi} \frac{4\pi}{2L + 1} r^{-\lambda-1} \sum_{M_L=-L}^{L} Y_{LM}^*(n_r) \int_{\mathbb{R}^3} d^3r' r^\lambda Y_{LM}(n'_r) j(r') \quad (\lambda = L, -L - 1).
\]  

(B.5)

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

\[
\sum_{m=-1}^{1} e_m^* e_m = 1
\]  

(B.6)

for the unit vectors of the cyclic basis, which gives

\[
A^{L\lambda}(r) = \frac{\mu_0}{4\pi} \frac{4\pi}{2L + 1} r^{-\lambda-1} \sum_{M_L=-L}^{L} \sum_{M_{L'}=-L}^{L} \sum_{m=-1}^{1} \sum_{m'=-1}^{1} Y_{LM}^*(n_r) e_m^* \int_{\mathbb{R}^3} d^3r' r^\lambda Y_{LM}(n'_r) e_m \cdot j(r')
\]  

(B.7)

\[
\langle L_{M_L} 1m | J M_J \rangle Y_{J M_J}^*(n_r) Y_{J M_J}(n_r) \quad (\lambda = L, -L - 1).
\]

The product \( Y_{LM}(n_r) e_m \), appearing in Eq. (B.7), may be expanded in the basis of vector spherical harmonics as

\[
Y_{LM}^*(n_r) e_m = \sum_{J=|L-1|}^{L+1} \sum_{M_J=-J}^{J} \langle L_{M_L} 1m | J M_J \rangle Y_{J M_J}^*(n_r) Y_{J M_J}(n_r).
\]  

(B.8)

Inserting this relation twice into Eq. (B.7) and exploiting the orthonormality property

\[
\sum_{M_a=-L_a}^{L_a} \sum_{M_b=-L_b}^{L_b} \langle L_a M_a L_b M_b | J M_J \rangle \langle L_a M_a L_b M_b | J' M_{J'} \rangle = \delta_{JJ'} \delta_{M_J M_{J'}}
\]  

(B.9)
of the Clebsch–Gordan coefficients yields

\[ A^{L\lambda}(r) = \frac{\mu_0}{4\pi} \frac{4\pi}{2L + 1} r^{-\lambda - 1} \sum_{J = |L - 1|}^{L + 1} \sum_{M_j = -J}^{J} Y_{JM_j}^L(n_r) \int_{\mathbb{R}^3} d^3r' r'^{\lambda} Y_{JM_j}^L(n'_r) \cdot j(r') \]

(\lambda = L, -L - 1). \quad (B.10)

If we define

\[ Z_{JM}^{L\lambda} = \sqrt{\frac{4\pi}{2L + 1}} \int_{\mathbb{R}^3} d^3r r^{\lambda} Y_{JM_j}^L(n_r) \cdot j(r) \quad (|L - 1| \leq J \leq L + 1), \quad (B.11) \]

Eq. (B.10) becomes

\[ A^{L\lambda}(r) = \frac{\mu_0}{4\pi} \sqrt{\frac{4\pi}{2L + 1}} r^{-\lambda - 1} \sum_{J = |L - 1|}^{L + 1} \sum_{M_j = -J}^{J} Z_{JM}^{L\lambda} Y_{JM_j}^L(n_r). \quad (B.12) \]

We shall show that the coefficients \( Z_{JM}^{L\lambda} \) are components of a rank-J irreducible spherical tensor \( Z_J^{L\lambda} \). Using the relation

\[ Y_{JM_j}^L(n_r) = \sum_{M_L = -L}^{L} \sum_{m = -1}^{1} (LM_L 1m | J M_J) Y_{LM_L}(n_r) e_m, \quad (B.13) \]

reciprocal to the one in Eq. (B.8), and the fact that the \( m \)-th cyclic component of the vector \( j(r) \) is given by

\[ j_m(r) = e_m \cdot j(r), \quad (B.14) \]

we obtain

\[ Y_{JM_j}^L(n_r) \cdot j(r) = \sum_{M_L = -L}^{L} \sum_{m = -1}^{1} (LM_L 1m | J M_J) Y_{LM_L}(n_r) j_m(r) = \{ Y_L(n_r) \otimes j(r) \}_{J M_J}, \quad (B.15) \]

and further

\[ Z_{JM}^{L\lambda} = \sqrt{\frac{4\pi}{2L + 1}} \int_{\mathbb{R}^3} d^3r r^{\lambda} \{ Y_L(n_r) \otimes j(r) \}_{J M_J}, \quad (B.16) \]

which proves the statement.

Concluding this section, we observe that since in the definition (B.11) \( J \) varies in the range \(|L - 1| \leq J \leq L + 1\), for \( L = 0 \) there are only two tensors in the \( Z_J^{L\lambda} \) family: \( Z_0^{L\lambda} \) and \( Z_0^{L+1,-1} \), while for \( L \geq 1 \) their number formally increases to six: \( Z_{L-1}^{LL}, Z_{L+1}^{LL}, Z_{L+1}^{L+1,L+1}, Z_{L-1}^{L+1,L-1}, Z_{L-1}^{L+1,-L-1}, Z_{L+1}^{L+1,-L-1} \). However, in Secs. (B.2) and (B.3) we shall show that the tensors \( Z_{L+1}^{LL} \) and \( Z_{L-1}^{L+1,-L-1} \) vanish identically.

**B.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. (B.3), with \( A^{LL}(r) \) given by Eq. (B.12) specialized to the case \( \lambda = L \). Components of the pertinent far-field tensors \( Z_{JM}^{LL} \) may be found from Eq. (B.11), in which one sets \( \lambda = L \).

Consider the tensor \( Z_{L+1,M_{L+1}}^{LL} \). In accordance with what has been said above, its components are given by

\[ Z_{L+1,M_{L+1}}^{LL} = \sqrt{\frac{4\pi}{2L + 1}} \int_{\mathbb{R}^3} d^3r r^{L} Y_{L+1,M_{L+1}}^L(n_r) \cdot j(r). \quad (B.17) \]
However, from the differential relation \[ Eq. (5.8.9) \]
\[
\nabla [(r^{\lambda+1}Y_{JM_j}(n_r))] = (J - \lambda - 1) \sqrt{\frac{J+1}{2J+1}} r^{J+1}Y_{JM_j}(n_r) + (J + \lambda + 2) \sqrt{\frac{J}{2J+1}} r^{J+1}Y_{JM_j}(n_r)
\]

it follows that
\[
r^L Y_{L+1,M_L+1}(n_r) = \frac{\nabla [r^{L+1}Y_{L+1,M_L+1}(n_r)]}{\sqrt{(L+1)(2L+3)}}.
\]

Consequently, the integrand in Eq. \[ Eq. (B.17) \] may be rewritten as
\[
r^L Y_{L+1,M_L+1}(n_r) \cdot j(r) = \frac{\nabla \cdot [r^{L+1}Y_{L+1,M_L+1}(n_r)]j(r)}{\sqrt{(L+1)(2L+3)}} = \frac{r^{L+1}Y_{L+1,M_L+1}(n_r) \nabla \cdot j(r)}{\sqrt{(L+1)(2L+3)}}.
\]

Since, by assumption, the current is solenoidal, the second term on the right-hand side of Eq. \[ Eq. (B.20) \] vanishes. Hence, replacing the integrand in Eq. \[ Eq. (B.17) \] by the first term on the right-hand side of Eq. \[ Eq. (B.20) \], and then using the Gauss divergence theorem, casts the former equation into
\[
Z^L_{L+1,M_L+1} = \frac{4\pi}{(L+1)(2L+1)(2L+3)} \lim_{r \to \infty} \int_{\partial R} d^2n_r \ r^{L+3}Y_{L+1,M_L+1}(n_r) n_r \cdot j(r).
\]

Hence, provided that the current obeys the asymptotic constraint
\[
\lim_{r \to \infty} r^{L+3}n_r \cdot j(r) = 0,
\]

one finds that
\[
Z^L_{L+1,M_L+1} = 0,
\]
i.e., the tensor \( Z^L_{L+1} \) vanishes identically. In result, Eqs. \[ Eq. (B.3) \] and \[ Eq. (B.12) \] may be combined into
\[
A(r) \rightarrow \infty \frac{\mu_0}{4\pi} \sum_{L=1}^{\infty} \frac{4\pi}{2L+1} r^{-L-1} \sum_{J=|L-1|}^{L} \sum_{M_L=-J}^{J} Z^L_{JM_L} Y_{JM_L}(n_r)
\]
(the sum starts from \( L = 1 \), as we have proved above that the tensor \( Z^{00} \) vanishes).

In the literature, instead of the tensors \( Z^L_{L} \) and \( Z^L_{L-1} \), one encounters the tensors \( M_L \) and \( T_{L-1} \), components of which, given by
\[
M_{LM_L} = -i \sqrt{\frac{4\pi L}{(L+1)(2L+1)}} \int_{\mathbb{R}^3} d^3r \ r^L Y_{L,M_L}(n_r) \cdot j(r)
\]

and
\[
T_{L-1,M_{L-1}} = - \frac{1}{2L+1} \sqrt{\frac{4\pi}{L}} \int_{\mathbb{R}^3} d^3r \ r^L Y_{L-1,M_{L-1}}(n_r) \cdot j(r),
\]

are related to those of \( Z^L_{L} \) and \( Z^{L-1}_{L-1} \) through
\[
M_{LM_L} = -i \sqrt{\frac{L}{L+1}} Z^L_{LM_L}
\]
and
\[
T_{L-1,M_{L-1}} = - \frac{1}{\sqrt{L(2L+1)}} Z^{L-1}_{L-1,M_{L-1}}.
\]

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 \[ \cite{10} \] (various integral representations of components of the \( 2^L \)-pole...
moment $\mathbf{T}_L$ are derived in Appendix C. With the use of components of these two more common tensors, the expansion (B.24) is replaced by

\[
A(r) \underset{r \to \infty}{\sim} \frac{\mu_0}{4\pi} \sum_{L=1}^{\infty} \sqrt{\frac{4\pi}{2L+1}} r^{-L-1} \left[ i \sqrt{\frac{L+1}{L}} \sum_{M_L=-L}^{L} \mathcal{M}_{LM_L} \mathbf{Y}^{L*}_{LM_L}(\mathbf{n}_r) 
- (1 - \delta_L) \sqrt{L(2L+1)} \sum_{M_{L-1}=-L+1}^{L-1} \mathcal{T}_{L-1,M_{L-1}} \mathbf{Y}^{L*}_{L-1,M_{L-1}}(\mathbf{n}_r) \right]. \tag{B.29}
\]

The factor $1 - \delta_L$ has been inserted into the second term in the square bracket since, as it will be 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

\[
B(r) = \nabla \times A(r). \tag{B.30}
\]

If we exploit the differential relation (B.18) with $\lambda = -L - 1$ and $J = L - 1$, this allows us to write the product $r^{-L-1} \mathbf{Y}^L_{L-1,M_{L-1}}(\mathbf{n}_r)$ as a gradient of a scalar field:

\[
r^{-L-1} \mathbf{Y}^L_{L-1,M_{L-1}}(\mathbf{n}_r) = \frac{\nabla [r^{-L} \mathbf{Y}^L_{L-1,M_{L-1}}(\mathbf{n}_r)]}{\sqrt{L(2L-1)}}. \tag{B.31}
\]

This immediately implies that

\[
\nabla \times [r^{-L-1} \mathbf{Y}^L_{L-1,M_{L-1}}(\mathbf{n}_r)] = \mathbf{0}. \tag{B.32}
\]

On the other hand, from the identity [38, Eq. (7.3.55)]

\[
\nabla \times [f(r) \mathbf{Y}^L_{LM_L}(\mathbf{n}_r)] = i \sqrt{\frac{L}{2L+1}} \left( \frac{\partial}{\partial r} - \frac{L}{r} \right) f(r) \mathbf{Y}^{L+1}_{LM_L}(\mathbf{n}_r)
+ i \sqrt{\frac{L+1}{2L+1}} \left( \frac{\partial}{\partial r} + \frac{L+1}{r} \right) f(r) \mathbf{Y}^{L-1}_{LM_L}(\mathbf{n}_r). \tag{B.33}
\]

one infers that

\[
\nabla \times [r^{-L-1} \mathbf{Y}^L_{LM_L}(\mathbf{n}_r)] = i \sqrt{L(2L+1)} r^{-L-2} \mathbf{Y}^{L+1}_{LM_L}(\mathbf{n}_r). \tag{B.34}
\]

On combining Eq. (B.30) with Eqs. (B.29), (B.32) and (B.34), one arrives at the sought asymptotic representation

\[
B(r) \underset{r \to \infty}{\sim} \frac{\mu_0}{4\pi} \sum_{L=1}^{\infty} \sqrt{4\pi(L+1)} r^{-L-2} \sum_{M_L=-L}^{L} \mathcal{M}_{LM_L} \mathbf{Y}^{L+1*}_{LM_L}(\mathbf{n}_r) \tag{B.35}
\]

of the magnetic induction. It is seen that components of the magnetic toroidal moments $\mathbf{T}_L$ do not appear in Eq. (B.35).

### B.3 The near-field case ($\lambda = -L - 1$). The tensors $\mathbf{N}_L$ and $\mathbf{U}_{L+1}$

In the near-field region, the asymptotic representation of the vector potential may be derived from Eqs. (B.4) and (B.12), the latter with $\lambda = -L - 1$. Components of the tensors $\mathbf{Z}^L_{L-1}$ are given by Eq. (B.11), with $\lambda$ specialized as above. Then, in complete analogy with what has been presented above, the use of the identity (B.31) leads to the inference that

\[
\mathbf{Z}^L_{L-1} = 0, \tag{B.36}
\]

provided that the current is constrained to obey

\[
\lim_{r \to 0} r^{-L+2} \mathbf{n}_r \cdot j(r) = 0. \tag{B.37}
\]
If, pursuing further the analogy with the material of Sec. B.2 we introduce the tensors $N_L$ and $U_{L+1}$ with components

$$N_{LM_L} = i \sqrt{\frac{4\pi (L+1)}{L (2L+1)}} \int_{\mathbb{R}^3} d^3 r \ r^{-L-1} Y^{L}_{LM_L}(n_r) \cdot j(r) \quad (B.38)$$

and

$$U_{L+1,M_L+1} = -\frac{1}{2L+1} \sqrt{\frac{4\pi}{L+1}} \int_{\mathbb{R}^3} d^3 r \ r^{-L-1} Y^{L}_{L+1,M_L+1}(n_r) \cdot j(r) \quad (B.39)$$

respectively, related to those of $Z^L_{L,-L-1}$ and $Z^L_{L+1}$ through

$$N_{LM_L} = i \sqrt{\frac{L+1}{L}} Z^{L,-L-1}_{LM_L} \quad (B.40)$$

and

$$U_{L+1,M_L+1} = -\frac{1}{\sqrt{(L+1)(2L+1)}} Z^{L,-L-1}_{L+1,M_L+1} \quad (B.41)$$

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

$$A(r) \xrightarrow{r \to 0} -\frac{\mu_0}{4\pi} \sum_{L=0}^{\infty} \sqrt{\frac{4\pi}{2L+1}} r^L \left[ (1 - \delta_{L0}) i \sqrt{\frac{L}{L+1}} \sum_{M_L=-L}^{L} N_{LM_L} Y^{L*}_{LM_L}(n_r) + \sqrt{(L+1)(2L+1)} \sum_{M_L=-L}^{L+1} U_{L+1,M_L+1} Y^{L*}_{L+1,M_L+1}(n_r) \right]. \quad (B.42)$$

The factor $1 - \delta_{L0}$ has been inserted into the first term in the square bracket since Eq. (B.12) implies that the only non-zero contribution to $A^{0,-1}(r)$ comes from the term involving components of the tensor $Z^0_{L,-1}$ [or equivalently, by virtue of Eq. (B.41), the tensor $U_1$].

The near-field multipole expansion of the magnetic induction is obtained from Eqs. (B.39) and (B.42) with the aid of the curl identities

$$\nabla \times [r^L Y^{L*}_{L+1,M_L+1}(n_r)] = 0 \quad (B.43)$$

[cf. Eq. (B.19)] and

$$\nabla \times [r^L Y^{L*}_{LM_L}(n_r)] = -i \sqrt{(L+1)(2L+1)} r^{L-1} Y^{L-1*}_{LM_L}(n_r) \quad (B.44)$$

[cf. Eq. (B.33)]. The required result is

$$B(r) \xrightarrow{r \to 0} -\frac{\mu_0}{4\pi} \sum_{L=1}^{\infty} \sqrt{4\pi} L r^{L-1} \sum_{M_L=-L}^{L} N_{LM_L} Y^{L-1*}_{LM_L}(n_r). \quad (B.45)$$

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 $j(r)$, spherical components of the magnetic toroidal 2$^L$-pole moment $T_L$ may be defined as

$$T_{LM} = -\frac{1}{2L+3} \sqrt{\frac{4\pi}{L+1}} \int_{\mathbb{R}^3} d^3 r \ r^{L+1} Y^{L+1}_{LM}(n_r) \cdot j(r), \quad (C.1)$$

The components of the magnetic toroidal multipole moments defined in Refs. [39,40] are complex conjugates of ours. Moreover, in Refs. [39,40] 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 $T_{LM}$. 


In the particular case \( \eta \) the expressions for \( T_L \) and \( T_M \) (observe that the irreducible tensor product appearing in the above equation is commutative).

Consider now the identity [38, Eq. (5.8.9)]

\[
\mathbf{Y}_{LM}(\mathbf{r}) = \frac{1}{4\pi L + 1} \int_{\mathbb{R}^3} d^3 \mathbf{r} \mathbf{r}^2 \frac{1}{2L + 1} \mathbf{Y}_{LM}(\mathbf{r}) \cdot \mathbf{j}(\mathbf{r})
\]

where \( \mathbf{Y}_{LM}(\mathbf{r}) \) denotes the vector spherical harmonic [B.13], or equivalently as

\[
T_{LM} = -\frac{1}{2L + 3} \sqrt{\frac{4\pi}{L + 1}} \int_{\mathbb{R}^3} d^3 \mathbf{r} \mathbf{r}^L + 1 \{ \mathbf{Y}_{L+1}(\mathbf{r}) \otimes \mathbf{j}(\mathbf{r}) \}_{LM}
\]

(C.2)

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

Hence, it follows that Eq. (C.1) may be rewritten as

\[
\mathbf{j}(\mathbf{r}) \cdot \mathbf{V}[f(\mathbf{r}) \mathbf{Y}_{LM}(\mathbf{r})] = -\sqrt{\frac{L + 1}{2L + 1}} \frac{\partial}{\partial r} \left( \frac{L}{r} \right) f(\mathbf{r}) \mathbf{Y}_{LM}^{L+1}(\mathbf{r})
\]

\[
+ \sqrt{\frac{L}{2L + 1}} \frac{\partial}{\partial r} \left( \frac{L + 1}{r} \right) f(\mathbf{r}) \mathbf{Y}_{LM}^{L-1}(\mathbf{r}).
\]

(C.3)

In the particular case \( f(\mathbf{r}) = r^{L+2} \), Eq. (C.3) yields

\[
\mathbf{j}(\mathbf{r}) \cdot \mathbf{V}[r^{L+2} \mathbf{Y}_{LM}(\mathbf{r})] = -2 \sqrt{\frac{L + 1}{2L + 1}} r^{L+1} \mathbf{Y}_{LM}^{L+1}(\mathbf{r}) + (2L + 3) \sqrt{\frac{L}{2L + 1}} r^L \mathbf{Y}_{LM}^{L-1}(\mathbf{r}).
\]

(C.4)

Hence, it follows that Eq. (C.1) may be rewritten as

\[
T_{LM} = \frac{\sqrt{\pi (2L + 1)}}{(L + 1)(2L + 3)} \int_{\mathbb{R}^3} d^3 \mathbf{r} \mathbf{j}(\mathbf{r}) \cdot \mathbf{V}[r^{L+2} \mathbf{Y}_{LM}(\mathbf{r})] - \frac{\sqrt{\pi L}}{L + 1} \int_{\mathbb{R}^3} d^3 \mathbf{r} r^{L+1} \mathbf{Y}_{LM}^{L-1}(\mathbf{r}) \cdot \mathbf{j}(\mathbf{r}).
\]

(C.5)

Let us transform the first integrand as follows:

\[
\mathbf{j}(\mathbf{r}) \cdot \mathbf{V}[r^{L+2} \mathbf{Y}_{LM}(\mathbf{r})] = \mathbf{j}(\mathbf{r}) \cdot [r^{L+2} \mathbf{Y}_{LM}(\mathbf{r}) \mathbf{j}(\mathbf{r})] - r^{L+2} \mathbf{Y}_{LM}(\mathbf{r}) \mathbf{V} \cdot \mathbf{j}(\mathbf{r}).
\]

(C.6)

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

\[
\lim_{r \to \infty} r^{L+4} \mathbf{n}_r \cdot \mathbf{j}(\mathbf{r}) = 0
\]

(C.7)

(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. (C.5) leads to the inference that the first integral on the right-hand side of Eq. (C.5) vanishes. In that way, we have proved that \( T_{LM} \), defined in Eq. (C.1) in terms of the vector harmonic \( \mathbf{Y}_{LM}^{L+1}(\mathbf{r}) \), may be equivalently expressed as

\[
T_{LM} = -\frac{\sqrt{\pi L}}{L + 1} \int_{\mathbb{R}^3} d^3 \mathbf{r} r^{L+1} \mathbf{Y}_{LM}^{L-1}(\mathbf{r}) \cdot \mathbf{j}(\mathbf{r}).
\]

(C.8)

Multiplying Eq. (C.8) by \( \eta \in \mathbb{C} \) and Eq. (C.1) by \( 1 - \eta \), and then adding, we find

\[
T_{LM} = -\frac{\sqrt{\pi L}}{2L + 1} \int_{\mathbb{R}^3} d^3 \mathbf{r} r^{L+1} \left[ \eta \sqrt{\frac{L}{L + 1}} \mathbf{Y}_{LM}^{L-1}(\mathbf{r}) + (1 - \eta) \frac{2}{2L + 3} \mathbf{Y}_{LM}^{L+1}(\mathbf{r}) \right] \cdot \mathbf{j}(\mathbf{r}).
\]

(C.9)

Playing with the value of \( \eta \), the above general formula may be used to obtain particular expressions for \( T_{LM} \), some of which have already appeared in the literature. For instance, with \( \eta = (L + 1)/(2L + 1) \), Eq. (C.9) becomes

\[
T_{LM} = -\frac{\sqrt{\pi L}}{2L + 1} \int_{\mathbb{R}^3} d^3 \mathbf{r} r^{L+1} \left[ \mathbf{Y}_{LM}^{L-1}(\mathbf{r}) + \frac{2}{2L + 3} \mathbf{Y}_{LM}^{L+1}(\mathbf{r}) \right] \cdot \mathbf{j}(\mathbf{r}),
\]

(C.10)

which coincides with Eq. (4.10) in Ref. [40]. Furthermore, if \( \eta = -2/(2L + 1) \), then Eq. (C.9) reduces to

\[
T_{LM} = \frac{1}{L + 1} \sqrt{\frac{4\pi}{2L + 1}} \int_{\mathbb{R}^3} d^3 \mathbf{r} r^{L+1} \left[ \mathbf{Y}_{LM}^{L-1}(\mathbf{r}) \right] - \frac{L + 1}{2L + 1} \mathbf{Y}_{LM}^{L+1}(\mathbf{r}) \cdot \mathbf{j}(\mathbf{r}).
\]

(C.11)
Since it is known (cf. Ref. [38, Eq. (7.3.70)]) that
\[
\sqrt{\frac{L}{2L+1}} Y^{L-1}_{LM}(n_r) - \sqrt{\frac{L+1}{2L+1}} Y^{L+1}_{LM}(n_r) = n_r Y_{LM}(n_r), \tag{C.12}
\]
Eq. (C.11) may be rewritten in the following compact form:
\[
T_{LM} = \frac{1}{L+1} \sqrt{\frac{4\pi}{2L+1}} \int_{\mathbb{R}^3} d^3r \, r^L Y_{LM}(n_r) r \cdot j(r), \tag{C.13}
\]
given before in Refs. [40, Eq. (B.4)] and [25, Eq. (2.2)]. The representation (C.13) of \(T_{LM}\) has been found to be most suitable for the purposes of this work, and the considerations presented in Sec. 5 have been based upon it. As the last example, in Eq. (C.9) we put
\[
\eta = \frac{2(L + 1)}{[(L + 2)/2L + 1]},
\]
This casts the latter equation into
\[
T_{LM} = \frac{-1}{L+1} \sqrt{\frac{4\pi L}{(L+1)(2L+1)}} \int_{\mathbb{R}^3} d^3r \, r^L Y_{LM}(n_r) r \cdot j(r), \tag{C.14}
\]
The integrand in Eq. (C.14) may be simplified with the aid of the formula (cf. Ref. [38, Eq. (7.3.73)])
\[
\sqrt{\frac{L}{2L+1}} Y^{L-1}_{LM}(n_r) + \sqrt{\frac{L}{2L+1}} Y^{L+1}_{LM}(n_r) = -i n_r \times Y^L_{LM}(n_r). \tag{C.15}
\]
This yields
\[
T_{LM} = \frac{-i}{L+1} \sqrt{\frac{4\pi L}{(L+1)(2L+1)}} \int_{\mathbb{R}^3} d^3r \, r^L Y^L_{LM}(n_r) \cdot [r \times j(r)], \tag{C.16}
\]
Since it holds that [38] Eqs. (7.3.9) and (7.3.6)]
\[
Y^L_{LM}(n_r) = \frac{\Lambda Y_{LM}(n_r)}{\sqrt{L+1}}, \tag{C.17}
\]
the third particular expression for \(T_{LM}\) we wish to present here is
\[
T_{LM} = \frac{i}{(L+1)(L+2)} \sqrt{\frac{4\pi}{2L+1}} \int_{\mathbb{R}^3} d^3r \, r^L Y_{LM}(n_r) \Lambda \cdot [r \times j(r)]. \tag{C.18}
\]
Concluding this appendix, we observe that the monopole toroidal moment vanishes identically. This is immediately seen if in Eq. (C.13) one sets \(L = M = 0\), obtaining
\[
T_{00} = \int_{\mathbb{R}^3} d^3r \, r \cdot j(r), \tag{C.19}
\]
and then one replaces the integrand by the right-hand side of the obvious identity
\[
r \cdot j(r) = \frac{1}{2} \nabla \cdot [r^2 j(r)] - \frac{1}{2} r^2 \nabla \cdot j(r). \tag{C.20}
\]

D Alternative integral representations of the near-field magnetic toroidal multipole moments \(U_L\)

In Appendix [3] we have come across a set of the near-nucleus magnetic toroidal multipole moments \(U_L\), with \(L \geq 1\), the spherical components of which are given by
\[
U_{LM} = -\frac{1}{2L-1} \sqrt{\frac{4\pi}{L}} \int_{\mathbb{R}^3} d^3r \, r^{-L} Y_{LM}^{L-1}(n_r) \cdot j(r), \tag{D.1}
\]
or equivalently by

\[ U_{LM} = -\frac{1}{2L - 1} \sqrt{\frac{4\pi}{L}} \int_{\mathbb{R}^3} d^3r \ r^{-L} \{ Y_{L-1}(n_r) \otimes j(r) \}_{LM}. \quad (D.2) \]

In this appendix, we aim to show that there is a one-parameter family of representations of \( U_{LM} \) which, under some constraints imposed on the current density \( j(r) \), are equivalent to the one given in Eq. (D.1). 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. (C.3) transforms the latter into

\[ \nabla [r^{-L+1} Y_{LM}(n_r)] = (2L - 1) \sqrt{\frac{L + 1}{2L - 1}} r^{-L} Y_{LM}^{L-1}(n_r) + 2 \sqrt{\frac{L}{2L - 1}} r^{-L} Y_{LM}^{L-1}(n_r), \quad (D.3) \]

hence, it follows that Eq. (D.1) may be rewritten as

\[ U_{LM} = -\frac{\sqrt{\pi(2L + 1)}}{L(2L - 1)} \int_{\mathbb{R}^3} d^3r \ j(r) \cdot \nabla [r^{-L+1} Y_{LM}(n_r)] + \frac{\sqrt{\pi(L + 1)}}{L} \int_{\mathbb{R}^3} d^3r \ r^{-L} Y_{LM}^{L+1}(n_r) \cdot j(r). \quad (D.4) \]

Now, it is evident that

\[ j(r) \cdot \nabla [r^{-L+1} Y_{LM}(n_r)] = \nabla \cdot [r^{-L+1} Y_{LM}(n_r) j(r)] - r^{-L+1} Y_{LM}(n_r) \nabla \cdot j(r). \quad (D.5) \]

Consequently, if the current is solenoidal and such that

\[ \lim_{r \to 0} r^{-L+3} n_r \cdot j(r) = 0, \quad \lim_{r \to \infty} r^{-L+3} n_r \cdot j(r) = 0, \quad (D.6) \]

the first integral on the right-hand side of Eq. (D.4) vanishes, yielding

\[ U_{LM} = \frac{\sqrt{\pi(L + 1)}}{L} \int_{\mathbb{R}^3} d^3r \ r^{-L} Y_{LM}^{L+1}(n_r) \cdot j(r). \quad (D.7) \]

Multiplying Eq. (D.1) by a parameter \( \eta \in \mathbb{C} \) and Eq. (D.7) by \( 1 - \eta \), and then adding, we obtain the sought one-parameter family of equivalent expressions

\[ U_{LM} = -\frac{\sqrt{\pi}}{L} \int_{\mathbb{R}^3} d^3r \ r^{-L} \left[ \frac{2}{2L - 1} Y_{LM}^{L-1}(n_r) - (1 - \eta) \sqrt{\frac{L + 1}{L}} Y_{LM}^{L+1}(n_r) \right] \cdot j(r), \quad (D.8) \]

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

Two particular choices of \( \eta \) are worth to be analyzed here. Thus, for

\[ \eta = \frac{2L - 1}{2L + 1}, \quad (D.9) \]

by virtue of the identity (C.12), we obtain

\[ U_{LM} = \frac{1}{L(L - 1)} \sqrt{\frac{4\pi}{2L + 1}} \int_{\mathbb{R}^3} d^3r \ r^{-L-1} Y_{LM}(n_r) r \cdot j(r), \quad (D.10) \]

while for

\[ \eta = \frac{(L + 1)(2L - 1)}{(L - 1)(2L + 1)} \quad (L \neq 1), \quad (D.11) \]

after exploiting the relations (C.15) and (C.17), we find

\[ U_{LM} = \frac{i}{L(L - 1)} \sqrt{\frac{4\pi}{2L + 1}} \int_{\mathbb{R}^3} d^3r \ r^{-L-1} Y_{LM}(n_r) \mathbf{A} \cdot [r \times j(r)] \quad (L \neq 1). \quad (D.12) \]
If \( L = 1 \) were admitted in Eq. (D.12), 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'Hopital's rule, we set \( L = 1 \) in the spherical harmonic and \( L = 1 + \varepsilon \) at other places in the above formula. Hence, if we let \( \varepsilon \) tend to zero, after exploiting the aforementioned rule, we obtain

\[
\hat{u}_{1M} = -i \sqrt{\frac{4\pi}{3}} \int_{\mathbb{R}^3} d^3r \, r^{-2} \ln(r/r_0) Y_{1M}(n_r) \mathbf{A} \cdot [\mathbf{r} \times j(r)],
\]

(D.13)

where \( r_0 \), of the physical dimension \( L \) 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

\[
I_{1M} = \int_{\mathbb{R}^3} d^3r \, r^{-2} Y_{1M}(n_r) \mathbf{A} \cdot [\mathbf{r} \times j(r)].
\]

(D.14)

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

\[
Y_{1M}(n_r) = \sqrt{\frac{3}{4\pi}} \frac{e_M \cdot n_r}{n_r \times e_M},
\]

(D.15)

the integral in Eq. (D.13) may be transformed into

\[
I_{1M} = \sqrt{\frac{3}{4\pi}} \int_{\mathbb{R}^3} d^3r \, r^{-3} [(\mathbf{r} \times \mathbf{A})(e_M \cdot \mathbf{r})] \cdot j(r).
\]

(D.16)

Hence, it follows that

\[
I_{1M} = -i \sqrt{\frac{3}{4\pi}} \int_{\mathbb{R}^3} d^3r \, \frac{n_r \times (n_r \times e_M)}{r} \cdot j(r).
\]

(D.17)

Now, it holds that

\[
\frac{n_r \times (n_r \times e_M)}{r} = -\nabla (e_M \cdot n_r),
\]

(D.18)

and consequently one has

\[
I_{1M} = i \sqrt{\frac{3}{4\pi}} \int_{\mathbb{R}^3} d^3r \, \nabla \cdot [(e_M \cdot n_r)j(r)] - i \sqrt{\frac{3}{4\pi}} \int_{\mathbb{R}^3} d^3r \, (e_M \cdot n_r) \nabla \cdot j(r).
\]

(D.19)

The first integral on the right-hand side is zero by virtue of the Gauss' theorem and the constraints in Eq. (D.6), while in the second one the integrand vanishes identically since, by assumption, the current is sourceless. This completes the proof.

### 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. 6 to 8, 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 \( \text{[41, Eq. (7.4.4.41)]} \)

\[
\, _3F_2 \left( \begin{array}{c} a, 1, 1 \\ b, 3 \end{array} ; 1 \right) = \frac{2(b - 1)}{a - 1} - \frac{2(b - 1)(b - a)}{(a - 1)(a - 2)} \left[ \psi(b - 1) - \psi(b - a + 1) \right] \quad [\text{Re}(b - a) > -1],
\]

(E.1)
which, after exploiting the relation
\[ \psi(z+1) = \psi(z) + \frac{1}{z}, \]  
(E.2)
may be transformed into
\[ 3F_2 \left( \begin{array}{c} a, 1, 1 \\ b, 3 \end{array} ; 1 \right) = \frac{2(b-1)}{a-2} - \frac{2(b-1)(b-a)}{(a-1)(a-2)} \psi(b-1) - \psi(b-a) \quad [\text{Re}(b-a) > -1]. \]
(E.3)

Below, we shall derive analogous expressions for the two remaining \(3F_2(1)\) functions of interest in the context of this work.

Playing with the definition
\[ 3F_2 \left( \begin{array}{c} a_1, a_2, a_3 \\ b_1, b_2 \end{array} ; z \right) = \frac{\Gamma(b_1)\Gamma(b_2) \sum_{n=0}^{\infty} \Gamma(n+a_1)\Gamma(n+a_2)\Gamma(n+a_3) z^n}{\Gamma(n+b_1)\Gamma(n+b_2)n!} \]
\[ ||z| \leq 1; \text{Re}(b_1 + b_2 - a_1 - a_2 - a_3) > 0 \text{ for } z = 1 \]  
(E.4)
(the constraints on \(z\), \(a\)'s and \(b\)'s will be tacitly assumed to hold throughout the rest of this appendix), it is possible to obtain the recurrence relation
\[ 3F_2 \left( \begin{array}{c} a_1, a_2, a_3 \\ b_1, b_2 \end{array} ; z \right) = \frac{a_3}{a_3-b_2+1} 3F_2 \left( \begin{array}{c} a_1, a_2, a_3+1 \\ b_1, b_2 \end{array} ; z \right) - \frac{b_2-1}{a_3-b_2+1} 3F_2 \left( \begin{array}{c} a_1, a_2, a_3 \\ b_1, b_2-1 \end{array} ; z \right), \]
(E.5)
from which we deduce that
\[ 3F_2 \left( \begin{array}{c} a, 1, 1 \\ b, n \end{array} ; 1 \right) = -\frac{1}{n-2} 3F_2 \left( \begin{array}{c} a, 1, 2 \\ b, n \end{array} ; 1 \right) + \frac{n-1}{n-2} 3F_2 \left( \begin{array}{c} a, 1, 1 \\ b, n-1 \end{array} ; 1 \right). \]
(E.6)

Next, we exploit the identity
\[ 3F_2 \left( \begin{array}{c} a_1, 1, a_3 \\ b_1, b_2 \end{array} ; z \right) = \frac{(b_1-1)(b_2-1)}{(a_1-1)(a_3-1)} 3F_2 \left( \begin{array}{c} a_1-1, 1, a_3-1 \\ b_1-1, b_2-1 \end{array} ; z \right) - \frac{(b_1-1)(b_2-1)}{(a_1-1)(a_3-1)}, \]
(E.7)
which also may be directly inferred from the definition (E.4). As the particular case of that identity, we have
\[ 3F_2 \left( \begin{array}{c} a, 1, 2 \\ b, n \end{array} ; 1 \right) = \frac{(n-1)(b-1)}{a-1} \frac{1}{3F_2 \left( \begin{array}{c} a, 1, 1 \\ b-1, n-1 \end{array} ; 1 \right)} - \frac{(n-1)(b-1)}{a-1}. \]
(E.8)

Insertion of Eq. (E.5) into Eq. (E.6) yields the relationship
\[ 3F_2 \left( \begin{array}{c} a, 1, 1 \\ b, n \end{array} ; 1 \right) = \frac{n-1}{n-2} 3F_2 \left( \begin{array}{c} a, 1, 1 \\ b, n-1 \end{array} ; 1 \right) - \frac{(n-1)(b-1)}{(n-2)(a-1)} 3F_2 \left( \begin{array}{c} a-1, 1, 1 \\ b-1, n-1 \end{array} ; 1 \right) + \frac{(n-1)(b-1)}{(n-2)(a-1)}. \]
(E.9)

If in Eq. (E.7) we put \(n = 4\), after simplifying the right-hand side with the use of Eqs. (E.3) and (E.2), we obtain
\[ 3F_2 \left( \begin{array}{c} a, 1, 1 \\ b, 4 \end{array} ; 1 \right) = \frac{3(b-1)(3a-2b-4)}{2(a-2)(a-3)} + \frac{3(b-1)(b-a)(b-a+1)}{(a-1)(a-2)(a-3)} [\psi(b-1) - \psi(b-a)] \quad [\text{Re}(b-a) > -2]. \]
(E.10)
Employing Eq. (E.9) recursively, in the similar manner we find

\[\begin{align*}
_3F_2\left( \begin{array}{c}
a, 1, 1 \\
b, 5 \\
1 
\end{array} ; 1 \right) &= \frac{2(b-1)(6b^2 + 24b - 15ab - 40a + 11a^2 + 36)}{3(a-2)(a-3)(a-4)} \\
&\quad - \frac{4(b-1)(b-a)(b-a+1)(b-a+2)}{(a-1)(a-2)(a-3)(a-4)} \left[\psi(b-1) - \psi(b-a)\right] \\
&\quad \text{[Re}(b-a) > -3]. \tag{E.11}
\end{align*}\]

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. (E.3), (E.10) and (E.11) are removable with an application of the L’Hospital’s rule.

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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 number in brackets following the entries is the power of 10 by which the entry is to be multiplied. 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 $\alpha^{-1}$ and, for the sake of making comparison with the results from Refs. [21, 22] more explicit, also its previous CODATA 2010 value.

| Source | $\alpha_1 (a_0^2)$ | $\alpha_2 (a_0^2)$ | $\alpha_3 (a_0^2)$ | $\alpha_4 (a_0^2)$ |
|--------|------------------|------------------|------------------|------------------|
| present (exact) | $4.499\,751\,495\,177\,875\,011\,523\,552$ | $1.499\,882\,982\,285\,755\,177\,470\,682\,(+1)$ | $1.312\,378\,214\,478\,562\,151\,040\,415\,(+2)$ | $2.126\,028\,674\,499\,338\,786\,454\,128\,(+3)$ |
| present (exact) | $\alpha^{-1} = 137.035\,999\,074$ (from CODATA 2010) | $1.499\,882\,982\,285\,644\,169\,960\,840\,(+1)$ | $1.312\,378\,214\,478\,446\,621\,510\,730\,(+2)$ | $2.126\,028\,674\,499\,128\,831\,459\,952\,(+3)$ |
| Ref. [21] | $4.499\,751\,495\,177\,639\,267\,396\,013$ | $1.499\,882\,982\,285\,644\,169\,960\,8\,(+1)$ | $1.312\,378\,214\,478\,446\,621\,510\,(+2)$ | $2.126\,028\,674\,499\,128\,831\,46\,(+3)$ |
| Ref. [22] | $4.499\,751\,495\,177\,639\,495\,177\,639\,267\,396\,02$ | $1.499\,882\,982\,285\,644\,169\,960\,8\,(+1)$ | $1.312\,378\,214\,478\,460\,(+2)$ | $2.126\,028\,674\,499\,147\,(+3)$ |
Table II: The static electric multipole polarizabilities $\alpha_L$ with $1 \leq L \leq 4$ for selected hydrogenic ions in the ground state, computed from the analytical formula in Eq. (3.41). The number in brackets following the entries is the power of 10 by which the entry is to be multiplied. The values of the inverse of the fine-structure constant used in calculations have been $\alpha^{-1} = 137.035\,999\,139$ (from CODATA 2014; results in the first row for each $Z$) and $\alpha^{-1} = 137.035\,999\,074$ (from CODATA 2010; results in the second row for each $Z$).

| $Z$ | $\alpha_1 (a_0^3)$ | $\alpha_2 (a_0^3)$ | $\alpha_3 (a_0^3)$ | $\alpha_4 (a_0^3)$ |
|-----|---------------------|---------------------|---------------------|---------------------|
| 1   | 4.499 751 495 177 875 011 524 (+0) | 4.499 882 982 285 755 177 471 (+1) | 1.312 378 214 478 562 151 040 (+2) | 2.126 028 649 499 338 786 454 (+3) |
| 2   | 2.111 877 749 177 639 256 396 (+0) | 5.125 050 375 239 509 639 311 (+1) | 2.075 546 062 025 167 458 (+0) | 2.075 546 061 205 188 564 (+0) |
| 3   | 7.190 661 246 047 167 462 734 (+3) | 9.581 265 372 341 791 023 296 (+4) | 3.352 210 608 794 400 804 905 (+5) | 2.171 618 426 950 907 701 171 (+4) |
| 4   | 4.475 164 360 648 818 455 398 (+4) | 1.488 319 833 924 471 652 035 (+5) | 1.300 352 899 799 117 538 323 (+6) | 2.104 187 645 771 176 667 402 (+7) |
| 5   | 2.750 523 499 121 230 880 495 (+5) | 2.271 146 583 119 162 558 714 (+7) | 4.938 640 072 445 973 751 899 (+9) | 1.991 062 443 096 913 712 558 (+10) |
| 6   | 1.604 002 839 692 739 227 002 (+6) | 3.218 326 876 777 344 766 036 (+9) | 1.717 671 116 979 420 309 765 (+11) | 1.707 067 336 752 410 153 201 (+13) |
| 7   | 2.797 090 475 043 278 635 137 (+7) | 2.371 147 053 789 055 379 606 (+10) | 5.443 579 082 362 361 630 978 (+13) | 2.345 208 225 059 515 662 725 (+15) |
| 8   | 7.256 230 366 973 582 550 880 (+8) | 3.196 013 750 479 081 681 921 (+11) | 3.921 694 890 318 033 520 828 (+14) | 9.141 660 900 197 762 990 639 (+17) |
| 9   | 7.256 230 363 582 213 484 281 (+8) | 3.196 013 748 838 032 427 240 (+11) | 3.921 694 887 293 335 137 309 (+14) | 9.141 660 892 322 525 362 993 (+17) |
| 10  | 2.168 647 589 558 746 030 622 (+8) | 5.405 559 190 506 306 646 268 (+12) | 3.923 335 160 173 613 355 838 (+15) | 5.514 202 255 886 621 078 935 (+18) |
| 11  | 2.168 647 587 493 674 593 651 (+8) | 5.405 559 183 469 571 103 004 (+12) | 3.923 335 154 079 824 764 316 (+15) | 5.514 202 246 346 336 408 556 (+18) |
| 12  | 5.962 322 886 341 222 518 228 (+9) | 3.850 889 829 402 244 690 391 (+13) | 3.675 741 125 180 401 231 657 (+16) | 3.240 357 008 255 786 619 282 (+19) |
| 13  | 5.962 322 872 671 608 906 403 (+9) | 3.850 889 803 174 165 102 275 (+13) | 3.675 741 111 635 729 711 889 (+16) | 3.240 356 994 994 515 555 786 (+19) |
| 14  | 5.748 648 400 700 781 043 837 (+10) | 3.159 735 442 958 334 459 896 (+14) | 6.689 221 528 538 828 261 530 (+18) | 3.139 717 909 213 994 303 355 (+21) |
| 15  | 5.748 647 780 061 286 039 034 (+10) | 3.159 734 965 737 634 785 405 (+14) | 6.689 220 281 323 310 175 469 (+18) | 3.139 717 224 793 817 462 022 (+21) |
Table III: Quasi-relativistic approximations for the static electric multipole polarizabilities $\alpha_L$ with $1 \leq L \leq 4$ for the Dirac one-electron atom in the ground state. The expressions have been derived from Eq. (3.51).

| $L$ | $\alpha_L$ |
|-----|-------------|
| 1   | $\frac{a_0^9}{Z^2} \frac{9}{2} \left[ 1 - \frac{28}{27} (\alpha Z)^2 \right]$ |
| 2   | $\frac{a_0^9}{Z^6} \frac{15}{15} \left[ 1 - \frac{293}{200} (\alpha Z)^2 \right]$ |
| 3   | $\frac{a_0^9}{Z^8} \frac{525}{4} \left[ 1 - \frac{5123}{2940} (\alpha Z)^2 \right]$ |
| 4   | $\frac{a_0^9}{Z^{10}} \frac{8505}{4} \left[ 1 - \frac{33251}{17010} (\alpha Z)^2 \right]$ |
Table IV: The static electric-to-magnetic multipole cross-susceptibilities $\alpha_{E \rightarrow M(L-1)}$ with $2 \leq L \leq 4$ for selected hydrogenic ions in the ground state, computed from the analytical formula in Eq. (4.42). The number in brackets following the entries is the power of 10 by which the entry is to be multiplied. The value of the inverse of the fine-structure constant used in calculations has been $\alpha^{-1} = 137.035999139$ (from CODATA 2014).

| $Z$ | $\alpha_{E2 \rightarrow M1}$ ($\alpha_0^1$) | $\alpha_{E3 \rightarrow M2}$ ($\alpha_0^2$) | $\alpha_{E4 \rightarrow M3}$ ($\alpha_0^3$) |
|-----|--------------------------------|--------------------------------|--------------------------------|
| 1   | 7.447 801 428 671 972 587 443 (−8) | 7.840 878 107 823 287 180 845 (−7) | 1.234 923 524 976 238 056 122 (−5) |
| 2   | 1.861 763 994 267 934 300 844 (−8) | 4.899 814 158 632 429 697 547 (−8) | 1.929 209 479 771 076 123 480 (−7) |
| 5   | 2.976 734 913 049 369 044 218 (−9) | 1.253 036 091 447 461 201 593 (−9) | 7.891 765 327 700 245 051 915 (−10) |
| 10  | 7.423 191 448 826 149 314 350 (−10) | 7.802 108 784 450 419 927 811 (−11) | 1.227 360 291 298 865 248 608 (−11) |
| 20  | 1.837 121 846 172 278 346 751 (−10) | 4.803 053 653 104 366 927 699 (−12) | 1.882 114 263 521 074 101 279 (−13) |
| 40  | 4.404 779 739 739 691 493 136 149 (−11) | 2.820 265 342 696 907 444 999 (−13) | 2.722 166 133 092 580 216 657 (−15) |
| 60  | 1.816 173 088 080 121 360 450 (−11) | 4.983 382 447 871 323 764 845 (−14) | 2.082 589 394 725 505 508 280 (−16) |
| 80  | 9.069 233 476 744 296 004 781 (−12) | 1.323 207 519 235 624 648 194 (−14) | 2.987 634 353 754 512 204 114 (−17) |
| 100 | 4.810 527 179 192 603 390 954 (−12) | 4.126 084 143 007 186 502 312 (−15) | 5.611 810 738 654 085 031 945 (−18) |
| 120 | 2.398 905 441 473 722 523 318 (−12) | 1.243 760 509 438 331 764 772 (−15) | 1.064 754 960 931 800 535 243 (−18) |
| 137 | 6.535 200 353 860 103 739 288 (−13) | 1.835 801 306 142 691 499 392 (−16) | 9.459 904 274 972 434 692 572 (−20) |
Table V: The static electric-to-magnetic multipole cross-susceptibilities $\alpha_{EL \rightarrow M(L+1)}$ with $1 \leq L \leq 4$ for selected hydrogenic ions in the ground state, computed from the analytical formula in Eq. (4.43). The number in brackets following the entries is the power of 10 by which the entry is to be multiplied. The value of the inverse of the fine-structure constant used in calculations has been $\alpha^{-1} = 137.035999139$ (from CODATA 2014).

| $Z$ | $\alpha_{E1 \rightarrow M2}$ ($a_{01}^0$) | $\alpha_{E2 \rightarrow M3}$ ($a_{02}^0$) | $\alpha_{E3 \rightarrow M4}$ ($a_{03}^0$) | $\alpha_{E4 \rightarrow M5}$ ($a_{04}^{10}$) |
|-----|---------------------------------|---------------------------------|---------------------------------|---------------------------------|
| 1   | 3.283609988211738758318 (−2)  | 1.641779910277485809376 (−1)  | 1.915387218714341770124 (−0)  | 3.878621704266776216353 (−1)  |
| 2   | 2.051888757574382373522 (−3)  | 2.564697947344304870341 (−3)  | 7.480041760822452355077 (−3)  | 3.786611359323821745607 (−2)  |
| 5   | 5.246149090038286019654 (−5)  | 1.048828974423698581549 (−5)  | 4.893086196104772001998 (−6)  | 3.962443793352933233712 (−6)  |
| 10  | 3.263961669540895253204 (−6)  | 1.629485276850519559523 (−7)  | 1.898813208632113003285 (−8)  | 3.841383757263664857256 (−9)  |
| 20  | 2.002912101253560623960 (−7)  | 2.488285199832601762511 (−9)  | 7.222989034894080541776 (−11) | 3.642467546249702021127 (−12) |
| 40  | 1.160561045666125723140 (−8)  | 3.536787823830012544234 (−11) | 2.529227814953036617056 (−13) | 3.150752599549890391915 (−15) |
| 60  | 2.001899182261258129378 (−9)  | 2.622080172857569638163 (−12) | 8.120641172461031595607 (−15) | 4.402352754592142514212 (−17) |
| 80  | 5.112923654383558308447 (−10)| 3.57687876504838084672 (−13) | 5.987127613932832469744 (−16) | 1.767496114114112526321 (−18) |
| 100 | 1.497342934870773796740 (−10)| 6.199237022887862992759 (−19) | 6.253163632400007961097 (−17) | 1.125356310598765215249 (−19) |
| 120 | 4.025596828302637918375 (−11)| 1.018161258743539778601 (−14) | 6.466767858953184265633 (−18) | 7.469936049505921356006 (−21) |
| 137 | 4.0952817093627479173 (−12)  | 5.745732037761833358905 (−16) | 2.193610026613034032245 (−19) | 1.601547888113102917378 (−22) |
Table VI: Quasi-relativistic approximations for the static electric-to-magnetic multipole cross-susceptibilities $\alpha_{EL\rightarrow M(L-1)}$ with $2 \leq L \leq 4$ and $\alpha_{EL\rightarrow M(L+1)}$ with $1 \leq L \leq 4$ for the Dirac one-electron atom in the ground state. The expressions have been derived from Eqs. (4.48) and (4.49).

| $L$  | $\alpha_{EL\rightarrow M(L-1)}$ | $\alpha_{EL\rightarrow M(L+1)}$ |
|------|-------------------------------|---------------------------------|
| 1    | $\frac{\alpha_a 9}{Z^4} \left[ 1 - \frac{409}{360} (\alpha Z)^2 \right]$ |                                  |
| 2    | $\frac{\alpha_a^4}{Z^4} \frac{23}{120} (\alpha Z)^2$ | $\frac{\alpha_a^6}{Z^6} \frac{45}{2} \left[ 1 \frac{1793}{1260} (\alpha Z)^2 \right]$ |
| 3    | $\frac{\alpha_a^6}{Z^6} \frac{113}{56} (\alpha Z)^2$ | $\frac{\alpha_a^8}{Z^8} \frac{525}{2} \left[ 1 \frac{3317}{2016} (\alpha Z)^2 \right]$ |
| 4    | $\frac{\alpha_a^8}{Z^8} \frac{1017}{32} (\alpha Z)^2$ | $\frac{\alpha_a^{10}}{Z^{10}} \frac{42525}{8} \left[ 1 \frac{759449}{415800} (\alpha Z)^2 \right]$ |
Table VII: The static electric-to-toroidal-magnetic multipole cross-susceptibilities $\alpha_{EL\rightarrow TL}$ with $1 \leq L \leq 4$ for selected hydrogenic ions in the ground state, computed from the analytical formula in Eq. (5.23). The number in brackets following the entries is the power of 10 by which the entry is to be multiplied. The value of the inverse of the fine-structure constant used in calculations has been $\alpha^{-1} = 137.035999139$ (from CODATA 2014).

| $Z$ | $\alpha_{E1\rightarrow T1}$ ($10^4$) | $\alpha_{E2\rightarrow T2}$ ($10^5$) | $\alpha_{E3\rightarrow T3}$ ($10^6$) | $\alpha_{E4\rightarrow T4}$ ($10^7$) |
|-----|---------------------------------|---------------------------------|---------------------------------|---------------------------------|
| 1   | 8.208 992 048 775 267 692 967 ($-3$) | 1.824 181 749 468 105 034 635 ($-2$) | 1.973 103 615 575 008 327 299 ($-1$) | 1.551 430 714 543 800 219 ($+0$) |
| 2   | 5.129 627 095 441 285 938 736 ($-4$) | 2.849 550 959 876 121 988 679 ($-4$) | 4.674 799 949 880 579 980 738 ($-4$) | 1.514 573 425 522 621 881 987 ($-3$) |
| 3   | 1.311 405 660 900 123 528 828 ($-5$) | 1.165 075 455 456 423 974 216 ($-6$) | 3.057 322 790 698 241 861 565 ($-7$) | 1.584 512 366 077 505 749 ($-7$) |
| 4   | 10.156 619 781 840 358 592 750 ($-7$) | 1.808 732 902 303 151 270 625 ($-8$) | 1.185 426 820 773 881 525 979 ($-9$) | 1.534 745 348 089 175 903 565 ($-10$) |
| 5   | 4.999 128 489 397 143 153 175 ($-8$) | 2.753 638 956 007 254 295 135 ($-10$) | 4.493 949 807 482 088 856 482 ($-12$) | 1.450 075 102 228 029 731 541 ($-13$) |
| 6   | 5.042 168 496 243 709 898 924 ($-10$) | 2.797 665 976 330 397 344 301 ($-13$) | 4.893 163 980 872 668 880 698 ($-16$) | 1.678 687 380 721 213 304 038 ($-18$) |
| 7   | 5.042 168 496 243 709 898 924 ($-10$) | 3.666 029 498 029 863 171 866 ($-14$) | 3.417 412 738 364 817 155 426 ($-16$) | 6.427 122 689 305 431 754 024 ($-20$) |
| 8   | 5.042 168 496 243 709 898 924 ($-10$) | 5.042 168 496 243 709 898 924 ($-11$) | 5.922 743 695 588 936 340 089 ($-15$) | 3.296 079 781 266 877 967 284 ($-18$) |
| 9   | 5.042 168 496 243 709 898 924 ($-10$) | 8.770 433 963 368 894 978 760 ($-12$) | 3.858 272 051 823 546 261 885 ($-15$) | 2.882 550 881 212 957 241 036 ($-19$) |
| 10  | 5.042 168 496 243 709 898 924 ($-10$) | 1.235 279 761 023 554 795 070 ($-11$) | 3.504 059 077 754 496 354 616 ($-16$) | 3.504 059 077 754 496 354 616 ($-11$) |
| 11  | 5.042 168 496 243 709 898 924 ($-10$) | 3.504 059 077 754 496 354 616 ($-11$) | 5.922 743 695 588 936 340 089 ($-15$) | 3.296 079 781 266 877 967 284 ($-18$) |
| 12  | 5.042 168 496 243 709 898 924 ($-10$) | 8.770 433 963 368 894 978 760 ($-12$) | 3.858 272 051 823 546 261 885 ($-15$) | 2.882 550 881 212 957 241 036 ($-19$) |
| 13  | 5.042 168 496 243 709 898 924 ($-10$) | 1.235 279 761 023 554 795 070 ($-11$) | 3.504 059 077 754 496 354 616 ($-16$) | 3.504 059 077 754 496 354 616 ($-11$) |
| 14  | 5.042 168 496 243 709 898 924 ($-10$) | 3.504 059 077 754 496 354 616 ($-11$) | 5.922 743 695 588 936 340 089 ($-15$) | 3.296 079 781 266 877 967 284 ($-18$) |
| 15  | 5.042 168 496 243 709 898 924 ($-10$) | 8.770 433 963 368 894 978 760 ($-12$) | 3.858 272 051 823 546 261 885 ($-15$) | 2.882 550 881 212 957 241 036 ($-19$) |
| 16  | 5.042 168 496 243 709 898 924 ($-10$) | 1.235 279 761 023 554 795 070 ($-11$) | 3.504 059 077 754 496 354 616 ($-16$) | 3.504 059 077 754 496 354 616 ($-11$) |
Table VIII: Quasi-relativistic approximations for the static electric-to-toroidal-magnetic multipole cross-susceptibilities $\alpha_{EL \rightarrow TL}$ with $1 \leq L \leq 4$ for the Dirac one-electron atom in the ground state. The expressions have been derived from Eq. (5.29).

| $L$ | $\alpha_{EL \rightarrow TL}$ |
|-----|-----------------------------|
| 1   | $\frac{\alpha_0^4}{Z^2} \frac{9}{8} \left[ 1 - \frac{785}{648} (\alpha Z)^2 \right]$ |
| 2   | $\frac{\alpha_0^6}{Z^5} \frac{5}{2} \left[ 1 - \frac{11591}{7200} (\alpha Z)^2 \right]$ |
| 3   | $\frac{\alpha_0^8}{Z^8} \frac{525}{32} \left[ 1 - \frac{654611}{352800} (\alpha Z)^2 \right]$ |
| 4   | $\frac{\alpha_0^{10}}{Z^{10}} \frac{1701}{8} \left[ 1 - \frac{8356217}{4082400} (\alpha Z)^2 \right]$ |
Table IX: Exact analytical expressions for the static electric multipole nuclear shielding constants $\sigma_{EL\to EL}$ with $1 \leq L \leq 4$ 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   | $\frac{1}{Z} \frac{104\gamma_1^2 + 110\gamma_1 - 79}{15(2\gamma_1 + 7)(4\gamma_1 - 1)}$ | $Z < \alpha^{-1} \sqrt{\frac{15}{4}}$ |
| 3   | $\frac{1}{Z} \frac{2064\gamma_1^4 + 14764\gamma_1^3 + 30968\gamma_1^2 + 7181\gamma_1 - 17177}{42(\gamma_1 + 7)(2\gamma_1 + 7)(4\gamma_1 + 11)(6\gamma_1 - 1)}$ | $Z < \alpha^{-1} \sqrt{\frac{35}{6}}$ |
| 4   | $\frac{1}{Z} \frac{14208\gamma_1^6 + 251184\gamma_1^5 + 1662556\gamma_1^4 + 4813404\gamma_1^3 + 5195413\gamma_1^2 - 862740\gamma_1 - 3136025}{90(\gamma_1 + 5)(\gamma_1 + 7)(2\gamma_1 + 5)(2\gamma_1 + 23)(4\gamma_1 + 11)(8\gamma_1 - 1)}$ | $Z < \alpha^{-1} \frac{3\sqrt{7}}{8}$ |
Table X: Quasi-relativistic approximations for static electric multipole shielding constants $\sigma_{E L \rightarrow E L}$ with $1 \leq L \leq 4$ for the Dirac one-electron atom in the ground state. The expressions have been derived from Eq. (6.27).

| $L$  | $\sigma_{E L \rightarrow E L}$                                                                 |
|------|---------------------------------------------------------------------------------------------|
| 1    | $\frac{1}{Z}$ (exact)                                                                     |
| 2    | $\frac{1}{Z^3} \left[ 1 - \frac{2}{5}(\alpha Z)^2 \right]$                                |
| 3    | $\frac{1}{Z^6} \left[ 1 - \frac{59}{84}(\alpha Z)^2 \right]$                            |
| 4    | $\frac{1}{Z^{10}} \left[ 1 - \frac{529}{540}(\alpha Z)^2 \right]$                       |
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 $\sigma_{EL\rightarrow M(L-1)}$ with $2 \leq L \leq 4$, 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 $\sigma_{EL\rightarrow M(L+1)}$ with $1 \leq L \leq 4$, obtained from Eq. (7.17) and given in the third column, remain valid.

| $L$ | $\sigma_{EL\rightarrow M(L-1)}$ | $\sigma_{EL\rightarrow M(L+1)}$ | constraint on $Z$
|-----|--------------------------------|--------------------------------|------------------|
| 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   | $\frac{\alpha a_0}{Z} \frac{3(2\gamma_1 + 1)(2\gamma_1 + 5)}{28(2\gamma_1 + 7)}$ | $\frac{\alpha Z}{a_0} \frac{50(32\gamma_1^4 + 164\gamma_1^3 - 53\gamma_1^2 - 84\gamma_1 - 231)}{189\gamma_1(\gamma_1 + 1)(\gamma_1 + 7)(8\gamma_1 - 1)(4\gamma_1 + 11)}$ | $Z < \alpha^{-1} \frac{3\sqrt{7}}{8}$ |
| 4   | $\frac{\alpha a_0}{Z} \frac{2(2\gamma_1 + 1)(68\gamma_1^2 + 483\gamma_1 + 709)}{315(\gamma_1 + 7)(4\gamma_1 + 11)}$ | $\frac{\alpha Z}{a_0} \frac{2(60\gamma_1^5 + 744\gamma_1^4 + 2065\gamma_1^3 - 964\gamma_1^2 - 5905\gamma_1 - 230)}{11\gamma_1(\gamma_1 + 1)(\gamma_1 + 5)(2\gamma_1 + 5)(2\gamma_1 + 23)(10\gamma_1 - 1)}$ | $Z < \alpha^{-1} \frac{3\sqrt{11}}{10}$ |
Table XII: Quasi-relativistic approximations for the near-nucleus static electric-to-magnetic multipole cross-susceptibilities $\sigma_{EL \rightarrow M(L-1)}$ with $2 \leq L \leq 4$ and $\sigma_{EL \rightarrow M(L+1)}$ with $1 \leq L \leq 4$ for the Dirac one-electron atom in the ground state. The expressions have been derived from Eqs. (7.24) and (7.25).

| $L$ | $\sigma_{EL \rightarrow M(L-1)}$ | $\sigma_{EL \rightarrow M(L+1)}$ |
|-----|---------------------------------|---------------------------------|
| 1   | $-\frac{aZ}{a_0} \frac{1}{3} \left[ 1 - \frac{1}{3} (\alpha Z)^2 \right]$ | $-\frac{a_0 4 Z}{5} \left[ 1 + \frac{25}{24} (\alpha Z)^2 \right]$ |
| 2   | $-\frac{aZ}{a_0} \frac{1}{3} \left[ 1 - \frac{1}{3} (\alpha Z)^2 \right]$ | $-\frac{a_0 8 Z}{35} \left[ 1 + \frac{223}{180} (\alpha Z)^2 \right]$ |
| 3   | $-\frac{aZ}{a_0} \frac{1}{4} \left[ 1 - \frac{23}{63} (\alpha Z)^2 \right]$ | $-\frac{a_0 20 Z}{189} \left[ 1 + \frac{1641}{1120} (\alpha Z)^2 \right]$ |
| 4   | $-\frac{aZ}{a_0} \frac{1}{5} \left[ 1 - \frac{1931}{5040} (\alpha Z)^2 \right]$ | $-\frac{a_0 2 Z}{33} \left[ 1 + \frac{10721}{6300} (\alpha Z)^2 \right]$ |

Table XIII: Exact analytical expressions for the near-nucleus static electric-to-magnetic-toroidal multipole cross-susceptibilities $\sigma_{EL \rightarrow TL}$ with $1 \leq L \leq 4$ 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 $Z < \alpha^{-1}$.

| $L$ | $\sigma_{EL \rightarrow TL}$ |
|-----|-----------------------------|
| 1   | $-\frac{a_0}{Z} \frac{1}{9} \left[ \frac{1}{\gamma_1} \left( \frac{1}{\gamma_1} + \frac{1}{\gamma_1} \right) + \frac{1}{\gamma_2} \frac{(2 \gamma_1 + 1)}{\gamma_2 + 1 + 3} \right] {}_3F_2\left( 1 \right.$ | $1, 1, \gamma_2 + 1, \gamma_2 + 1 + 1 \left. ; 1 \right)$ |
| 2   | $-\frac{a_0}{Z} \frac{1}{20} \frac{(2 \gamma_1 + 1)(2 \gamma_1 + 3)}{2 \gamma_1 + 7}$ |
| 3   | $-\frac{a_0}{Z} \frac{1}{21} \frac{(\gamma_1 + 1)(2 \gamma_1 + 1)(4 \gamma_1^2 + 34 \gamma_1 + 67)}{(\gamma_1 + 7)(2 \gamma_1 + 7)(4 \gamma_1 + 11)}$ |
| 4   | $-\frac{a_0}{Z} \frac{1}{216} \frac{(48 \gamma_1^5 + 1092 \gamma_1^4 + 8856 \gamma_1^3 + 31625 \gamma_1^2 + 48384 \gamma_1 + 23395)}{(\gamma_1 + 5)(\gamma_1 + 7)(2 \gamma_1 + 5)(2 \gamma_1 + 23)(4 \gamma_1 + 11)}$ |
Table XIV: The near-nucleus static electric-to-toroidal-magnetic dipole cross-susceptibilities \( \sigma_{E1\rightarrow T1} \) for selected hydrogenic ions in the ground state, computed from Eq. (8.16) with \( L = 1 \). The number in brackets following the entries is the power of 10 by which the entry is to be multiplied. The value of the inverse of the fine-structure constant used in calculations has been \( \alpha^{-1} = 137.035999139 \) (from CODATA 2014).

| \( Z \) | \( \sigma_{E1\rightarrow T1} (a_0) \) |
|-------|-------------------------------|
| 1     | \(-3.648\ 637\ 095\ 595\ 566\ 551\ 586 \times 10^{-3}\) |
| 2     | \(-1.824\ 259\ 765\ 869\ 242\ 452\ 438 \times 10^{-3}\) |
| 5     | \(-7.295\ 393\ 076\ 288\ 932\ 910\ 227 \times 10^{-4}\) |
| 10    | \(-3.644\ 756\ 614\ 282\ 248\ 624\ 473 \times 10^{-4}\) |
| 20    | \(-1.816\ 493\ 443\ 607\ 184\ 794\ 164 \times 10^{-4}\) |
| 40    | \(-8.964\ 422\ 142\ 806\ 221\ 802\ 427 \times 10^{-5}\) |
| 60    | \(-5.844\ 669\ 492\ 463\ 283\ 200\ 203 \times 10^{-5}\) |
| 80    | \(-4.246\ 284\ 894\ 885\ 672\ 771\ 322 \times 10^{-5}\) |
| 100   | \(-3.264\ 717\ 305\ 265\ 228\ 591\ 534 \times 10^{-5}\) |
| 120   | \(-2.646\ 549\ 207\ 670\ 313\ 520\ 251 \times 10^{-5}\) |
| 137   | \(-1.413\ 712\ 752\ 786\ 307\ 100\ 801 \times 10^{-4}\) |

Table XV: Quasi-relativistic approximations for the near-nucleus static electric-to-toroidal-magnetic multipole cross-susceptibilities \( \sigma_{EL\rightarrow TL} \) with \( 1 \leq L \leq 4 \) 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 \( 2 \leq L \leq 4 \) have been derived from Eq. (8.21).

| \( L \) | \( \sigma_{EL\rightarrow TL} \) |
|-------|-----------------------------|
| 1     | \(-\frac{\alpha a_0}{Z} \left[ 1 - \left( \frac{3}{4} - \frac{\pi^2}{18} \right) (\alpha Z)^2 \right] \) |
| 2     | \(-\frac{\alpha a_0}{Z} \left[ 1 - \frac{19}{45} (\alpha Z)^2 \right] \) |
| 3     | \(-\frac{\alpha a_0}{Z} \left[ 1 - \frac{343}{720} (\alpha Z)^2 \right] \) |
| 4     | \(-\frac{\alpha a_0}{Z} \left[ 1 - \frac{113623}{226800} (\alpha Z)^2 \right] \) |
Table XVI: The collection of formulas defining the multipole susceptibilities considered in the present paper.

| susceptibility       | related induced moment | constraints |
|----------------------|-------------------------|-------------|
| \( \alpha_{EL\rightarrow EL} \) | \( Q_L^{(1)} = (4\pi\epsilon_0)\alpha_{EL\rightarrow EL} C_L^{(1)} \) | far-field zone |
| \( \alpha_{EL\rightarrow MA} \) | \( M^{(1)} = (4\pi\epsilon_0)c\alpha_{EL\rightarrow MA} \frac{\nu \otimes C_L^{(1)}}{\langle 10L0|\lambda0 \rangle} \) | \( \lambda = \begin{cases} 2 & \text{for } L = 1 \\ L \mp 1 & \text{for } L \geq 2 \end{cases} \) |
| \( \alpha_{EL\rightarrow TL} \) | \( T_L^{(1)} = i(4\pi\epsilon_0)c\alpha_{EL\rightarrow TL} \sqrt{L(L+1)} \{ \nu \otimes C_L^{(1)} \} L \) | near-nucleus zone |
| \( \sigma_{EL\rightarrow EL} \) | \( R_L^{(1)} = (4\pi\epsilon_0)\sigma_{EL\rightarrow EL} C_L^{(1)} \) |
| \( \sigma_{EL\rightarrow MA} \) | \( N^{(1)} = (4\pi\epsilon_0)c\sigma_{EL\rightarrow MA} \frac{\nu \otimes C_L^{(1)}}{\langle 10L0|\lambda0 \rangle} \) | \( \lambda = \begin{cases} 2 & \text{for } L = 1 \\ L \mp 1 & \text{for } L \geq 2 \end{cases} \) |
| \( \sigma_{EL\rightarrow TL} \) | \( U_L^{(1)} = i(4\pi\epsilon_0)c\sigma_{EL\rightarrow TL} \sqrt{L(L+1)} \{ \nu \otimes C_L^{(1)} \} L \) |
Table XVII: The table shows how the susceptibilities studied in the present paper enter the near- and far-zone asymptotic representations of static electric $\mathbf{E}^{(1)}(r)$ and magnetic $\mathbf{B}^{(1)}(r)$ fields, and of their potentials: scalar $\phi^{(1)}(r)$ and vector $\mathbf{A}^{(1)}(r)$, 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 $(L \geq 1)$ electric field $E_L^{(1)}(r)$ derivable from the scalar potential $\varphi_L^{(1)}(r)$ defined in Eq. (2.1).

| induced field | near-zone representation | far-zone representation |
|--------------|--------------------------|-------------------------|
| $\phi^{(1)}(r)$ | $\sigma_{\text{EL} \rightarrow \text{EL}} \sqrt{\frac{4\pi}{2L+1}} r^L \sum_{M=-L}^{L} C_{LM}^{(1)} Y_M^*(n_r) = -\sigma_{\text{EL} \rightarrow \text{EL}} \varphi_L^{(1)}(r)$ | $\alpha_{\text{EL} \rightarrow \text{EL}} \sqrt{\frac{4\pi}{2L+1}} r^{-L-1} \sum_{M=-L}^{L} C_{LM}^{(1)} Y_M^*(n_r)$ |
| $\mathbf{E}^{(1)}(r)$ | $-\sigma_{\text{EL} \rightarrow \text{EL}} \sqrt{4\pi r^L} r^{-L-1} \sum_{M=-L}^{L} C_{LM}^{(1)} Y_L^{(-1)*}(n_r) = -\sigma_{\text{EL} \rightarrow \text{EL}} \mathbf{E}_L^{(1)}(r)$ | $-\alpha_{\text{EL} \rightarrow \text{EL}} \sqrt{4\pi (L+1) r^{-L-2}} \sum_{M=-L}^{L} C_{LM}^{(1)} \mathbf{Y}_L^{-1*}(n_r)$ |
| $\mathbf{A}^{(1)}(r)$ | $-\sum_{\lambda=L}^{L+1} \frac{i \epsilon}{\sigma_{\text{EL} \rightarrow \text{EL}}} (1 - \delta_{00}) \sqrt{\frac{4\pi}{(L+1)(2L+1)}} r^{\lambda} \sum_{\mu=-\lambda}^{\lambda} \frac{\langle \nu \otimes \mathcal{C}_L^{(1)} \rangle_{LM} Y_{-\lambda}^{(1)*}(n_r)}{(10L0)\lambda 0}$ | $\sum_{\lambda=L+1}^{\lambda\sigma} \frac{i \epsilon}{\sigma_{\text{EL} \rightarrow \text{EL}}} (1 - \delta_{00}) \sqrt{\frac{4\pi (\lambda + 1)}{(\lambda(2\lambda+1))}} r^{-\lambda-1} \sum_{\mu=-\lambda}^{\lambda} \frac{\langle \nu \otimes \mathcal{C}_L^{(1)} \rangle_{LM} Y_{-\lambda}^{(1)*}(n_r)}{(10L0)\lambda 0}$ |
| $\mathbf{B}^{(1)}(r)$ | $-\sum_{\lambda=L}^{L+1} \frac{c}{\sigma_{\text{EL} \rightarrow \text{EL}}} (1 - \delta_{00}) \sqrt{\frac{4\pi}{(L+1)^2}} r^{\lambda-1} \sum_{\mu=-\lambda}^{\lambda} \frac{\langle \nu \otimes \mathcal{C}_L^{(1)} \rangle_{LM} Y_{-\lambda}^{(1)*}(n_r)}{(10L0)\lambda 0}$ | $-\sum_{\lambda=L+1}^{\lambda\sigma} \frac{c}{\sigma_{\text{EL} \rightarrow \text{EL}}} (1 - \delta_{00}) \sqrt{\frac{4\pi (\lambda + 1)}{(\lambda(2\lambda+1))}} r^{-\lambda-2} \sum_{\mu=-\lambda}^{\lambda} \frac{\langle \nu \otimes \mathcal{C}_L^{(1)} \rangle_{LM} Y_{-\lambda}^{(1)*}(n_r)}{(10L0)\lambda 0}$ |
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 $\alpha_{E\to L} \equiv \alpha_{L}$, the electric-to-magnetic cross-susceptibilities $\alpha_{E\to M(L+1)}$ and the electric-to-toroidal-magnetic cross-susceptibility $\alpha_{E\to TL}$. All the formulas are valid for $L \geq 1$ and under the constraint $Z < \alpha^{-1}$.

\[ \alpha_{E\to L} = \frac{a_0^{2L+1}}{Z^{2L+2}} \frac{\Gamma(2\gamma_L + 2L + 2)}{2^{2L}L(L+1)(2L+1)\Gamma(2\gamma_L + 1)} \times \left\{ \frac{1}{2} + \frac{L^2(L+1)^2(\gamma_L + 1)^2(\gamma_L + 1 + L + 1)}{(2L + 1)(\gamma_L - 1 + 1)\Gamma(2\gamma_L + 2L + 2)\Gamma(2\gamma_L + 1)} \right\} F_2 \left( \begin{array}{c} \gamma_L - 1 - L, \gamma_L - 1 - L, \gamma_L - 1 + 1 ; 1 \\ \gamma_L - 1 + 2, 2\gamma_L + 1 \end{array} \right) \]

\[ \alpha_{E\to M(L-1)} = \frac{a_0^{2L}}{Z^{2L}} \frac{(L-1)\Gamma(2\gamma_L + 2L + 1)}{2^{2L-1}(L+1)(4L^2 - 1)\Gamma(2\gamma_L + 1)} \times \left\{ \frac{1}{2} - \frac{2L(L+1)(\gamma_L - 1 + 1)\Gamma(2\gamma_L + 2L + 1 + 1)}{(\gamma_L - 1 + 1)\Gamma(2\gamma_L + 2L + 1)\Gamma(2\gamma_L + 1)} \right\} F_2 \left( \begin{array}{c} \gamma_L - 1 - L, \gamma_L - 1 - L, \gamma_L - 1 + 1 ; 1 \\ \gamma_L - 1 + 2, 2\gamma_L + 1 \end{array} \right) \]

\[ \alpha_{E\to M(L+1)} = \frac{a_0^{2L+2}}{Z^{2L+2}} \frac{(L+1)\Gamma(2\gamma_L + 2L + 3)}{2^{2L+1}(L+1)(2L+1)(2L+3)\Gamma(2\gamma_L + 1)} \times \left\{ \frac{1}{2} + \frac{(L+2)(\gamma_L - 1)\Gamma(2\gamma_L + 2L + 1 + 1)\Gamma(2\gamma_L + 2L + 2)}{(L+1)(\gamma_L - 1 + 1)\Gamma(2\gamma_L + 2L + 1)\Gamma(2\gamma_L + 1)} \right\} F_2 \left( \begin{array}{c} \gamma_L + 1 - 1 - L, \gamma_L + 1 - 1 - L, \gamma_L + 1 - 1 + 1 ; 1 \\ \gamma_L + 1 - 1 + 2, 2\gamma_L + 1 \end{array} \right) \]

\[ \alpha_{E\to TL} = \frac{a_0^{2L+2}}{Z^{2L+2}} \frac{1}{2^{2L+1}(2L+1)^2\Gamma(2\gamma_L + 1)} \left\{ \frac{\Gamma(2\gamma_L + 2L + 1)\Gamma(\gamma_L + 1 + L + 1)}{(\gamma_L - 1 + 1)\Gamma(2\gamma_L + 1)} \right\} F_2 \left( \begin{array}{c} \gamma_L - 1 - L, \gamma_L - 1 - L, \gamma_L - 1 + 1 ; 1 \\ \gamma_L - 1 + 2, 2\gamma_L + 1 \end{array} \right) \]

+ \frac{[L(\gamma_L - 1) - 1]\Gamma(2\gamma_L + 2L + 1 + 1)\Gamma(2\gamma_L + 2L + 2)}{(L+1)(\gamma_L + 1 - L)\Gamma(2\gamma_L + 1)} \right\} F_2 \left( \begin{array}{c} \gamma_L + 1 - 1 - L, \gamma_L + 1 - 1 - L, \gamma_L + 1 - 1 + 1 ; 1 \\ \gamma_L + 1 - 1 + 2, 2\gamma_L + 1 \end{array} \right) \]
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 $\sigma_{E \rightarrow E}$, the electric-to-magnetic cross-susceptibilities $\sigma_{E \rightarrow M(L+1)}$ and the electric-to-toroidal-magnetic cross-susceptibility $\sigma_{E \rightarrow T}$. All the formulas hold for $L \geq 1$, except for the one for $\sigma_{E \rightarrow M(L-1)}$, which makes physical sense only for $L \geq 2$.

| Susceptibility | Constraints |
|----------------|-------------|
| $\sigma_{E \rightarrow E}$ | $Z < \alpha^{-1}$ for $L = 1$ |
| $\sigma_{E \rightarrow M(L-1)}$ | $L \geq 2$; $Z < \alpha^{-1}$ |
| $\sigma_{E \rightarrow T}$ | $Z < \alpha^{-1}$ |

$$
\sigma_{E \rightarrow E} = \frac{2}{Z(L+1)(2L+1)} \left\{ 1 + \frac{L^2(L+1)(\gamma_1+1)\gamma(L+1)-L}{(2L+1)(\gamma_2+1)(\gamma_2+L-L)} \right\} 3F_2 \left( \begin{array}{c} -L+1, 1, \gamma_2 - \gamma_1 - L \\ \gamma_2 - \gamma_1 + 2, \gamma_2 + \gamma_1 - L + 1 \end{array} ; 1 \right) \\
- \frac{L(L+1)^2(\gamma_1+1)[L(\gamma_1-1)-1]}{(2L+1)(\gamma_{L+1}+\gamma_1-L)} 3F_2 \left( \begin{array}{c} -L+1, 1, \gamma_{L+1} - \gamma_1 - L \\ \gamma_{L+1} - \gamma_1 + 2, \gamma_{L+1} + \gamma_1 - L + 1 \end{array} ; 1 \right)
$$

$$
\sigma_{E \rightarrow M(L-1)} = \frac{\alpha Z}{\gamma L(2L+1)(2L+3)} \left\{ 1 - \frac{(L+1)^2(\gamma_1-1)}{(\gamma_{L+1}+\gamma_1+L+1)(\gamma_{L+1}+\gamma_1-L-1)} \right\} 3F_2 \left( \begin{array}{c} -L+1, 1, \gamma_{L+1} - \gamma_1 - L \\ \gamma_{L+1} - \gamma_1 + 2, \gamma_{L+1} + \gamma_1 - L + 1 \end{array} ; 1 \right)
$$

$$
\sigma_{E \rightarrow T} = -\frac{\alpha_0 Z}{\gamma L(2L+1)(2L+3)} \left\{ \frac{\gamma_1+1}{L(\gamma_1-1)} \right\} 3F_2 \left( \begin{array}{c} -L+2, 1, \gamma_2 - \gamma_1 - L \\ \gamma_2 - \gamma_1 + 2, \gamma_2 + \gamma_1 - L + 2 \end{array} ; 1 \right)
$$

$$
+ \frac{L(\gamma_1-1)-1}{(L+1)(\gamma_{L+1}+\gamma_1+L+1)} 3F_2 \left( \begin{array}{c} -L+2, 1, \gamma_{L+1} - \gamma_1 - L \\ \gamma_{L+1} - \gamma_1 + 2, \gamma_{L+1} + \gamma_1 - L + 2 \end{array} ; 1 \right)
$$