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Gordon decomposition of the static dipole polarizability of the relativistic hydrogen-like atom: application of the Sturmian expansion of the first-order Dirac–Coulomb Green function

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Abstract

The Sturmian expansion of the generalized first-order Dirac–Coulomb Green function (Szmytkowski 1997 *J. Phys. B: At. Mol. Opt. Phys.* **30** 825, 2747) is used to derive an analytical formula for the static dipole polarizability of the relativistic hydrogen-like atom in the ground state. The formula contains a generalized hypergeometric series ${}_3F_2$ with the unit argument. It is identical with one found recently, in a completely different way, by Yakhontov (2003 *Phys. Rev. Lett.* **91** 093001) and is the most compact among all known analytical expressions for the polarizability. Partitioning of the polarizability into convection and spin-polarization components, resulting from the Gordon decomposition of an induced electronic charge density, is carried out. It appears that the spin-polarization component of the polarizability vanishes.

1. Introduction

Shortly after Dirac's discovery of a wave equation for a relativistic electron, Gordon [1] proposed an ingenious procedure for partitioning relativistic electrons' probability and current densities into so-called convection, spin-polarization and, in the latter case, spin-magnetization components. To some extent, this partitioning has its counterpart in the structure of electric charge and current densities in the Maxwell–Lorentz electromagnetic theory of continuous media [2].

Over several decades, Gordon's result was considered primarily as an interesting trifle and was used mainly for educational purposes. Only recently, Pyper [3–7] and Szmytkowski [8, 9] have illustrated its practical utility, partitioning various *magnetic* properties of relativistic atomic systems into their dia- and paramagnetic components. In this paper, we exploit the Gordon procedure to decompose, into convection and spin-polarization parts, the fundamental *electric* property of a relativistic hydrogen-like atom: a static dipole polarizability of the ground state.

The structure of the paper is as follows. In section 2 we summarize relevant facts from the first-order perturbation theory for the ground state of the relativistic hydrogen-like atom in a static homogeneous electric field. A compact analytical expression for the ground state static electric dipole polarizability of the relativistic hydrogen-like atom, identical with that found recently, in a completely different way, by Yakhontov [10], is derived in section 3. The Gordon decomposition of the polarizability is carried out in section 4. Calculations in sections 3 and 4 exploit the Sturmian expansion of the generalized first-order Dirac–Coulomb Green function [11, 12, 9]. Brief conclusions are given in section 5. The paper ends with an appendix discussing some relevant properties of the generalized hypergeometric function ${}_3F_2$ appearing in sections 3 and 4.

2. A relativistic hydrogen-like atom in a weak static uniform electric field

The energy quasi-eigenvalue problem for quasi-bound states of a relativistic hydrogen-like atom, with an infinitely heavy, point-like and spinless nucleus of charge $+Ze$, placed in a weak static uniform electric field $\boldsymbol{F} = F\boldsymbol{n}_z$ ($\boldsymbol{n}_z$ is the unit vector along the z-axis of a Cartesian coordinate system), is constituted by the Dirac equation

$$\left[-\mathrm{i}c\hbar\boldsymbol{\alpha}\cdot\boldsymbol{\nabla} + \beta mc^2 - \frac{Ze^2}{(4\pi\epsilon_0)r} + e\boldsymbol{F}\cdot\boldsymbol{r} - E\right]\psi(\boldsymbol{r}) = 0 \qquad (2.1)$$

(here $\boldsymbol{\alpha}$ and β are the standard 4×4 Dirac matrices [13]), supplemented by the boundary conditions

$$r\psi(\boldsymbol{r}) \xrightarrow{r\to 0} 0, \qquad r\psi(\boldsymbol{r}) \xrightarrow{r\to\infty} 0. \qquad (2.2)$$

In virtue of our assumption that the electric field is weak, the interaction potential

$$V^{(1)}(\boldsymbol{r}) = e\boldsymbol{F}\cdot\boldsymbol{r} \qquad (2.3)$$

may be considered as a small perturbation of the zeroth-order Hamiltonian describing an isolated atom. The zeroth-order bound state eigenproblem is constituted by the Dirac–Coulomb equation

$$\left[-\mathrm{i}c\hbar\boldsymbol{\alpha}\cdot\boldsymbol{\nabla} + \beta mc^2 - \frac{Ze^2}{(4\pi\epsilon_0)r} - E^{(0)}\right]\psi^{(0)}(\boldsymbol{r}) = 0, \qquad (2.4)$$

supplemented by the boundary conditions

$$r\psi^{(0)}(\boldsymbol{r}) \xrightarrow{r\to 0} 0, \qquad r\psi^{(0)}(\boldsymbol{r}) \xrightarrow{r\to\infty} 0. \qquad (2.5)$$

In the rest of the work, we shall restrict ourselves to the case when the unperturbed state of the atom is the ground state. Then one has

$$E^{(0)} = mc^2\gamma_1, \qquad (2.6)$$

where

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

with $\alpha = e^2/(4\pi\epsilon_0)c\hbar$ (not to be confused with the Dirac matrix $\boldsymbol{\alpha}$ or the polarizability α_{d}) being the Sommerfeld fine-structure constant. The eigenvalue $E^{(0)}$ is doubly degenerate.

Two orthonormal eigenfunctions to the problem (2.4) and (2.5) associated with $E^{(0)}$ are, for instance,

$$\psi_M^{(0)}(\boldsymbol{r}) = \frac{1}{r}\begin{pmatrix} P^{(0)}(r)\,\Omega_{-1M}(\boldsymbol{n}_r) \\ \mathrm{i}Q^{(0)}(r)\,\Omega_{+1M}(\boldsymbol{n}_r)\end{pmatrix}, \tag{2.8}$$

with $M = \pm 1/2$. Here $\Omega_{\kappa\mu}(\boldsymbol{n}_r)$, with $\boldsymbol{n}_r = \boldsymbol{r}/r$, is a spherical spinor, while the radial functions are

$$P^{(0)}(r) = -\sqrt{\frac{Z}{a_0}\frac{1+\gamma_1}{\Gamma(2\gamma_1+1)}}\left(\frac{2Zr}{a_0}\right)^{\gamma_1}\exp(-Zr/a_0) \tag{2.9}$$

and

$$Q^{(0)}(r) = \sqrt{\frac{Z}{a_0}\frac{1-\gamma_1}{\Gamma(2\gamma_1+1)}}\left(\frac{2Zr}{a_0}\right)^{\gamma_1}\exp(-Zr/a_0), \tag{2.10}$$

with $a_0 = (4\pi\epsilon_0)\hbar^2/me^2$ denoting the Bohr radius. The functions (2.8) are eigenfunctions, associated with the eigenvalues $M\hbar$, of the projection $\hat{J}_z$ of the total angular momentum on the direction of the perturbing electric field.

Since both the Hamiltonian of an isolated atom and the perturbing potential $V^{(1)}(\boldsymbol{r})$ commute with the operator $\hat{J}_z$, the perturbation does not mix states associated with different eigenvalues of $\hat{J}_z$. Consequently, the perturbation-adjusted zeroth-order eigenfunctions are those in equation (2.8).

We shall seek approximate solutions to the eigenproblem (2.1) and (2.2) in the form

$$\psi_M(\boldsymbol{r}) \simeq \psi_M^{(0)}(\boldsymbol{r}) + \psi_M^{(1)}(\boldsymbol{r}), \qquad E_M \simeq E^{(0)} + E_M^{(1)}. \tag{2.11}$$

The corrections $\psi_M^{(1)}(\boldsymbol{r})$ and $E_M^{(1)}$, which, by assumption, are small quantities of the first order in F, are solutions to the inhomogeneous problem

$$\left[-\mathrm{i}c\hbar\boldsymbol{\alpha}\cdot\boldsymbol{\nabla} + \beta mc^2 - \frac{Ze^2}{(4\pi\epsilon_0)r} - E^{(0)}\right]\psi_M^{(1)}(\boldsymbol{r}) = -\left[e\boldsymbol{F}\cdot\boldsymbol{r} - E_M^{(1)}\right]\psi_M^{(0)}(\boldsymbol{r}), \tag{2.12}$$

$$r\psi_M^{(1)}(\boldsymbol{r}) \xrightarrow{r\to 0} 0, \qquad r\psi_M^{(1)}(\boldsymbol{r}) \xrightarrow{r\to\infty} 0. \tag{2.13}$$

Henceforth, we shall assume that

$$\int_{\mathbb{R}^3} \mathrm{d}^3\boldsymbol{r}\; \psi_M^{(0)\dagger}(\boldsymbol{r})\psi_{M'}^{(1)}(\boldsymbol{r}) = 0. \tag{2.14}$$

In the standard way, from equation (2.12) we obtain

$$E_M^{(1)} = e\boldsymbol{F}\cdot\int_{\mathbb{R}^3} \mathrm{d}^3\boldsymbol{r}\; \psi_M^{(0)\dagger}(\boldsymbol{r})\boldsymbol{r}\psi_M^{(0)}(\boldsymbol{r}) \tag{2.15}$$

and

$$\psi_M^{(1)}(\boldsymbol{r}) = -\int_{\mathbb{R}^3} \mathrm{d}^3\boldsymbol{r}'\; \mathcal{G}^{(0)}(\boldsymbol{r},\boldsymbol{r}')\left[e\boldsymbol{F}\cdot\boldsymbol{r}' - E_M^{(1)}\right]\psi_M^{(0)}(\boldsymbol{r}'), \tag{2.16}$$

where $\mathcal{G}^{(0)}(\boldsymbol{r},\boldsymbol{r}')$ is the *generalized* (or *reduced*) Dirac–Coulomb Green function for the energy level $E^{(0)}$. It is a solution to the inhomogeneous differential equation ($\boldsymbol{r}'$ fixed)

$$\begin{aligned}&\left[-\mathrm{i}c\hbar\boldsymbol{\alpha}\cdot\boldsymbol{\nabla} + \beta mc^2 - \frac{Ze^2}{(4\pi\epsilon_0)r} - E^{(0)}\right]\mathcal{G}^{(0)}(\boldsymbol{r},\boldsymbol{r}') \\ &\qquad = \mathcal{I}\delta^3(\boldsymbol{r}-\boldsymbol{r}') - \sum_{M'=\pm 1/2}\psi_{M'}^{(0)}(\boldsymbol{r})\psi_{M'}^{(0)\dagger}(\boldsymbol{r}')\end{aligned} \tag{2.17}$$

(here $\mathcal{I}$ is the unit 4×4 matrix) with the boundary conditions

$$r\mathcal{G}^{(0)}(\boldsymbol{r}, \boldsymbol{r}') \stackrel{r\to 0}{\longrightarrow} 0, \qquad r\mathcal{G}^{(0)}(\boldsymbol{r}, \boldsymbol{r}') \stackrel{r\to \infty}{\longrightarrow} 0, \tag{2.18}$$

and obeys the additional orthogonality constraints

$$\int_{\mathbb{R}^3} \mathrm{d}^3\boldsymbol{r}'\, \mathcal{G}^{(0)}(\boldsymbol{r}, \boldsymbol{r}')\psi^{(0)}_{\pm 1/2}(\boldsymbol{r}') = 0. \tag{2.19}$$

The latter constraints imply that equation (2.16) may be simplified to

$$\psi^{(1)}_M(\boldsymbol{r}) = -eF \int_{\mathbb{R}^3} \mathrm{d}^3\boldsymbol{r}'\, \mathcal{G}^{(0)}(\boldsymbol{r}, \boldsymbol{r}')\boldsymbol{n}_z \cdot \boldsymbol{r}'\psi^{(0)}_M(\boldsymbol{r}'). \tag{2.20}$$

Henceforth, for brevity, we shall suppress the subscripts M at wavefunctions and energies.

3. Direct evaluation of the polarizability

The dipole atomic polarizability α_{d} is defined through the relationship

$$\alpha_{\mathrm{d}} = \frac{1}{(4\pi\epsilon_0)} \frac{\boldsymbol{F} \cdot \boldsymbol{p}^{(1)}}{F^2}, \tag{3.1}$$

where

$$\boldsymbol{p}^{(1)} = \int_{\mathbb{R}^3} \mathrm{d}^3\boldsymbol{r}\, \boldsymbol{r}\rho^{(1)}(\boldsymbol{r}) \tag{3.2}$$

is an *induced* electric dipole moment of an atom in the perturbed state $\psi(\boldsymbol{r})$. In equation (3.2), $\rho^{(1)}(\boldsymbol{r})$ is a first-order contribution to an induced electronic charge density in the state $\psi(\boldsymbol{r})$, given by

$$\rho^{(1)}(\boldsymbol{r}) = -e\psi^{(1)\dagger}(\boldsymbol{r})\psi^{(0)}(\boldsymbol{r}) - e\psi^{(0)\dagger}(\boldsymbol{r})\psi^{(1)}(\boldsymbol{r}) = -2e\,\mathrm{Re}\,\psi^{(0)\dagger}(\boldsymbol{r})\psi^{(1)}(\boldsymbol{r}). \tag{3.3}$$

On substituting equation (3.3) into (3.2), we obtain

$$\boldsymbol{p}^{(1)} = -2e\,\mathrm{Re} \int_{\mathbb{R}^3} \mathrm{d}^3\boldsymbol{r}\, \psi^{(0)\dagger}(\boldsymbol{r})\boldsymbol{r}\psi^{(1)}(\boldsymbol{r}), \tag{3.4}$$

hence, after utilizing equation (2.20), we arrive at

$$\alpha_{\mathrm{d}} = \frac{2e^2}{(4\pi\epsilon_0)} \int_{\mathbb{R}^3} \mathrm{d}^3\boldsymbol{r} \int_{\mathbb{R}^3} \mathrm{d}^3\boldsymbol{r}'\, \psi^{(0)\dagger}(\boldsymbol{r})\boldsymbol{n}_z \cdot \boldsymbol{r}\mathcal{G}^{(0)}(\boldsymbol{r}, \boldsymbol{r}')\boldsymbol{n}_z \cdot \boldsymbol{r}'\psi^{(0)}(\boldsymbol{r}'). \tag{3.5}$$

Here, we have omitted the symbol Re since the double integral is evidently real.

Equation (3.5) may be simplified by using the following series representation of the generalized Dirac–Coulomb Green function

$$\mathcal{G}^{(0)}(\boldsymbol{r}, \boldsymbol{r}') = \frac{(4\pi\epsilon_0)}{e^2} \sum_{\substack{\kappa=-\infty \\ (\kappa\neq 0)}}^{\infty} \sum_{m=-|\kappa|+1/2}^{|\kappa|-1/2} \frac{1}{rr'} \times \begin{pmatrix} g^{(0)}_{(++)\kappa}(r, r')\Omega_{\kappa m}(\boldsymbol{n}_r)\Omega^{\dagger}_{\kappa m}(\boldsymbol{n}'_r) & -\mathrm{i}g^{(0)}_{(+-)\kappa}(r, r')\Omega_{\kappa m}(\boldsymbol{n}_r)\Omega^{\dagger}_{-\kappa m}(\boldsymbol{n}'_r) \\ \mathrm{i}g^{(0)}_{(-+)\kappa}(r, r')\Omega_{-\kappa m}(\boldsymbol{n}_r)\Omega^{\dagger}_{\kappa m}(\boldsymbol{n}'_r) & g^{(0)}_{(--)\kappa}(r, r')\Omega_{-\kappa m}(\boldsymbol{n}_r)\Omega^{\dagger}_{-\kappa m}(\boldsymbol{n}'_r) \end{pmatrix} \tag{3.6}$$

and the known relation

$$\boldsymbol{n}_z \cdot \boldsymbol{n}_r\Omega_{\kappa m}(\boldsymbol{n}_r) = -\frac{2m}{4\kappa^2 - 1}\Omega_{-\kappa m}(\boldsymbol{n}_r) + \frac{\sqrt{\left(\kappa + \frac{1}{2}\right)^2 - m^2}}{|2\kappa + 1|}\Omega_{\kappa+1,m}(\boldsymbol{n}_r) + \frac{\sqrt{\left(\kappa - \frac{1}{2}\right)^2 - m^2}}{|2\kappa - 1|}\Omega_{\kappa-1,m}(\boldsymbol{n}_r). \tag{3.7}$$

Carrying out angular integrations in equation (3.5), with the aid of equations (3.6) and (3.7), one finds that the polarizability may be written in the form

$$\alpha_{\mathrm{d}} = \alpha_{\mathrm{d},+1} + \alpha_{\mathrm{d},-2}, \tag{3.8}$$

with

$$\alpha_{\mathrm{d},+1} = \frac{2}{9}\int_0^\infty \mathrm{d}r \int_0^\infty \mathrm{d}r'\, rr' \begin{pmatrix} P^{(0)}(r) & Q^{(0)}(r) \end{pmatrix} \mathsf{G}_{+1}^{(0)}(r,r') \begin{pmatrix} P^{(0)}(r') \\ Q^{(0)}(r') \end{pmatrix} \tag{3.9}$$

and

$$\alpha_{\mathrm{d},-2} = \frac{4}{9}\int_0^\infty \mathrm{d}r \int_0^\infty \mathrm{d}r'\, rr' \begin{pmatrix} P^{(0)}(r) & Q^{(0)}(r) \end{pmatrix} \mathsf{G}_{-2}^{(0)}(r,r') \begin{pmatrix} P^{(0)}(r') \\ Q^{(0)}(r') \end{pmatrix}. \tag{3.10}$$

The 2×2 matrices

$$\mathsf{G}_{\kappa}^{(0)}(r,r') = \begin{pmatrix} g_{(++)\kappa}^{(0)}(r,r') & g_{(+-)\kappa}^{(0)}(r,r') \\ g_{(-+)\kappa}^{(0)}(r,r') & g_{(--)\kappa}^{(0)}(r,r') \end{pmatrix} \qquad (\kappa = +1, -2), \tag{3.11}$$

appearing in equations (3.9) and (3.10) are the symmetry-adapted radial generalized Dirac–Coulomb Green functions for the energy level $E^{(0)}$. Since none of the two values assumed by κ in equation (3.11) coincides with -1 (which is the value of κ characterizing the zeroth-order eigenstates (2.8)), the functions (3.11) have the following Sturmian expansions [11]:

$$\mathsf{G}_{\kappa}^{(0)}(r,r') = \sum_{n=-\infty}^{\infty} \frac{1}{\mu_{n\kappa}^{(0)} - 1} \begin{pmatrix} S_{n\kappa}^{(0)}(r) \\ T_{n\kappa}^{(0)}(r) \end{pmatrix} \begin{pmatrix} \mu_{n\kappa}^{(0)} S_{n\kappa}^{(0)}(r') & T_{n\kappa}^{(0)}(r') \end{pmatrix} \qquad (\kappa = +1, -2), \tag{3.12}$$

where

$$\mu_{n\kappa}^{(0)} = \frac{|n| + \gamma_\kappa + N_{n\kappa}}{\gamma_1 + 1}, \tag{3.13}$$

$$S_{n\kappa}^{(0)}(r) = \sqrt{\frac{(1+\gamma_1)(|n|+2\gamma_\kappa)|n|!}{2ZN_{n\kappa}(N_{n\kappa}-\kappa)\Gamma(|n|+2\gamma_\kappa)}} \times \left(\frac{2Zr}{a_0}\right)^{\gamma_\kappa} \mathrm{e}^{-Zr/a_0} \left[L_{|n|-1}^{(2\gamma_\kappa)}\left(\frac{2Zr}{a_0}\right) + \frac{\kappa - N_{n\kappa}}{|n| + 2\gamma_\kappa} L_{|n|}^{(2\gamma_\kappa)}\left(\frac{2Zr}{a_0}\right) \right], \tag{3.14}$$

and

$$T_{n\kappa}^{(0)}(r) = \sqrt{\frac{(1-\gamma_1)(|n|+2\gamma_\kappa)|n|!}{2ZN_{n\kappa}(N_{n\kappa}-\kappa)\Gamma(|n|+2\gamma_\kappa)}} \times \left(\frac{2Zr}{a_0}\right)^{\gamma_\kappa} \mathrm{e}^{-Zr/a_0} \left[L_{|n|-1}^{(2\gamma_\kappa)}\left(\frac{2Zr}{a_0}\right) - \frac{\kappa - N_{n\kappa}}{|n| + 2\gamma_\kappa} L_{|n|}^{(2\gamma_\kappa)}\left(\frac{2Zr}{a_0}\right) \right] \tag{3.15}$$

($L_n^{(\alpha)}(\rho)$ is the generalized Laguerre polynomial [14]; we define $L_{-1}^{(\alpha)}(\rho) \equiv 0$). The 'apparent principal quantum number' $N_{n\kappa}$, appearing in equations (3.13)–(3.15), is defined as

$$N_{n\kappa} = \pm\sqrt{(|n| + \gamma_\kappa)^2 + (\alpha Z)^2} = \pm\sqrt{|n|^2 + 2|n|\gamma_\kappa + \kappa^2} \tag{3.16}$$

(note that $N_{n\kappa}$ may assume positive as well as negative values!). The following sign convention is adopted in the definition (3.16): the plus sign should be chosen for $n > 0$ and the minus one for $n < 0$; for $n = 0$ one chooses the plus sign if $\kappa < 0$ and the minus sign if $\kappa > 0$.

The radial integrals, resulting after substituting the expansions (3.12) into equations (3.9) and (3.10), may be evaluated with the aid of the known formula [15]

$$\int_0^\infty \mathrm{d}\rho\, \rho^\alpha \mathrm{e}^{-\rho} L_n^{(\beta)}(\rho) = \frac{\Gamma(\alpha+1)\Gamma(n+\beta-\alpha)}{n!\Gamma(\beta-\alpha)} \qquad (\mathrm{Re}\,\alpha > -1). \tag{3.17}$$

Then, reducing terms with the same $|n|$ to a common denominator, with no difficulty one obtains

$$\alpha_{\mathrm{d},+1} = \frac{a_0^3}{Z^4} \frac{\gamma_1(\gamma_1+1)(2\gamma_1+1)(4\gamma_1+5)}{36} \tag{3.18}$$

and, after rather laborious calculations, exploiting the Gauss formula

$${}_2F_1\left(\begin{matrix} a_1, a_2 \\ b \end{matrix}; 1\right) = \frac{\Gamma(b)\Gamma(b-a_1-a_2)}{\Gamma(b-a_1)\Gamma(b-a_2)} \qquad (\mathrm{Re}\,(b-a_1-a_2) > 0) \tag{3.19}$$

and the definition (A.1),

$$\begin{aligned} \alpha_{\mathrm{d},-2} = \frac{a_0^3}{Z^4}\bigg[& -\frac{(\gamma_1+1)(2\gamma_1+1)(2\gamma_1+3)\big(4\gamma_1^4-8\gamma_1^3-25\gamma_1^2-4\gamma_1+27\big)}{9(4\gamma_1+1)^2} \\ & + \frac{(\gamma_1-2)^2\Gamma^2(\gamma_1+\gamma_2+2)}{6(\gamma_2-\gamma_1)(\gamma_2-\gamma_1-2)^2\Gamma(2\gamma_1+1)\Gamma(2\gamma_2+1)} \\ & \times {}_3F_2\left(\begin{matrix} \gamma_2-\gamma_1-2, \gamma_2-\gamma_1-2, \gamma_2-\gamma_1 \\ \gamma_2-\gamma_1+1, 2\gamma_2+1 \end{matrix}; 1\right)\bigg], \end{aligned} \tag{3.20}$$

where ${}_3F_2$ is the generalized hypergeometric series. Hence, one finds

$$\begin{aligned} \alpha_{\mathrm{d}} = \frac{a_0^3}{Z^4}\bigg[& -\frac{(\gamma_1+1)(2\gamma_1+1)\big(32\gamma_1^5-80\gamma_1^4-408\gamma_1^3-376\gamma_1^2+163\gamma_1+324\big)}{36(4\gamma_1+1)^2} \\ & + \frac{(\gamma_1-2)^2\Gamma^2(\gamma_1+\gamma_2+2)}{6(\gamma_2-\gamma_1)(\gamma_2-\gamma_1-2)^2\Gamma(2\gamma_1+1)\Gamma(2\gamma_2+1)} \\ & \times {}_3F_2\left(\begin{matrix} \gamma_2-\gamma_1-2, \gamma_2-\gamma_1-2, \gamma_2-\gamma_1 \\ \gamma_2-\gamma_1+1, 2\gamma_2+1 \end{matrix}; 1\right)\bigg]. \end{aligned} \tag{3.21}$$

The right-hand sides of equations (3.20) and (3.21) may be simplified if one employs the following recurrence relation derived in appendix A:

$$\begin{aligned} {}_3F_2\left(\begin{matrix} a_1, a_2, a_3 \\ a_3+1, b \end{matrix}; 1\right) = {} & \frac{\Gamma(b)\Gamma(b-a_1-a_2)}{\Gamma(b-a_1)\Gamma(b-a_2)}\left[1 + \frac{a_1 a_2}{(b-a_1-a_2-1)(b-a_3-1)}\right] \\ & - \frac{a_1 a_2}{(a_3+1)(b-a_3-1)}\, {}_3F_2\left(\begin{matrix} a_1+1, a_2+1, a_3+1 \\ a_3+2, b \end{matrix}; 1\right) \\ & (\mathrm{Re}\,(b-a_1-a_2) > 1). \end{aligned} \tag{3.22}$$

Application of this relation transforms equations (3.20) and (3.21) into

$$\begin{aligned} \alpha_{\mathrm{d},-2} = \frac{a_0^3}{Z^4}\bigg[& \frac{(\gamma_1+1)(2\gamma_1+1)(2\gamma_1+3)}{9} - \frac{(\gamma_1-2)^2\Gamma^2(\gamma_1+\gamma_2+2)}{18(\gamma_2-\gamma_1+1)\Gamma(2\gamma_1+1)\Gamma(2\gamma_2+1)} \\ & \times {}_3F_2\left(\begin{matrix} \gamma_2-\gamma_1-1, \gamma_2-\gamma_1-1, \gamma_2-\gamma_1+1 \\ \gamma_2-\gamma_1+2, 2\gamma_2+1 \end{matrix}; 1\right)\bigg] \end{aligned} \tag{3.23}$$

and

$$\begin{aligned} \alpha_{\mathrm{d}} = \frac{a_0^3}{Z^4}\bigg[& \frac{(\gamma_1+1)(2\gamma_1+1)\big(4\gamma_1^2+13\gamma_1+12\big)}{36} - \frac{(\gamma_1-2)^2\Gamma^2(\gamma_1+\gamma_2+2)}{18(\gamma_2-\gamma_1+1)\Gamma(2\gamma_1+1)\Gamma(2\gamma_2+1)} \\ & \times {}_3F_2\left(\begin{matrix} \gamma_2-\gamma_1-1, \gamma_2-\gamma_1-1, \gamma_2-\gamma_1+1 \\ \gamma_2-\gamma_1+2, 2\gamma_2+1 \end{matrix}; 1\right)\bigg], \end{aligned} \tag{3.24}$$

respectively. Recently, Yakhontov [10] arrived at the result in equation (3.24) following a route completely different from ours.

In the nonrelativistic limit

$$\gamma_1 \overset{c\to\infty}{\longrightarrow} 1, \qquad \gamma_2 \overset{c\to\infty}{\longrightarrow} 2 \tag{3.25}$$

and the generalized hypergeometric series in equation (3.24) reduces to

$${}_3F_2\left(\begin{matrix}0,0,2\\3,5\end{matrix};1\right) = 1. \tag{3.26}$$

Hence, one reproduces the well-known (cf [13], section 33) result

$$\alpha_{\mathrm{d}} \overset{c\to\infty}{\longrightarrow} \frac{9}{2}\frac{a_0^3}{Z^4}. \tag{3.27}$$

4. Gordon decomposition of the polarizability

The electronic charge density in the perturbed state $\psi(\boldsymbol{r})$ is

$$\rho(\boldsymbol{r}) = -e\psi^\dagger(\boldsymbol{r})\psi(\boldsymbol{r}), \tag{4.1}$$

or, equivalently,

$$\rho(\boldsymbol{r}) = -\tfrac{1}{2}e\psi^\dagger(\boldsymbol{r})\psi(\boldsymbol{r}) - \tfrac{1}{2}e\psi^\dagger(\boldsymbol{r})\psi(\boldsymbol{r}). \tag{4.2}$$

From equation (2.1) one has

$$\psi(\boldsymbol{r}) = \frac{E - V^{(0)}(r) - V^{(1)}(\boldsymbol{r})}{mc^2}\beta\psi(\boldsymbol{r}) + \frac{\mathrm{i}\hbar}{mc}\beta\boldsymbol{\alpha}\cdot\boldsymbol{\nabla}\psi(\boldsymbol{r}), \tag{4.3}$$

with

$$V^{(0)}(\boldsymbol{r}) = -\frac{Ze^2}{(4\pi\epsilon_0)r} \tag{4.4}$$

and with $V^{(1)}(\boldsymbol{r})$ defined in equation (2.3). On substituting the expression (4.3) and its Hermitian conjugate into, respectively, the first and the second terms on the right-hand side of equation (4.2), one arrives at the following Gordon decomposition of the density $\rho(\boldsymbol{r})$:

$$\rho(\boldsymbol{r}) = \rho_{\mathrm{c}}(\boldsymbol{r}) + \rho_{\mathrm{p}}(\boldsymbol{r}), \tag{4.5}$$

with

$$\rho_{\mathrm{c}}(\boldsymbol{r}) = -e\frac{E - V^{(0)}(r) - V^{(1)}(\boldsymbol{r})}{mc^2}\psi^\dagger(\boldsymbol{r})\beta\psi(\boldsymbol{r}) \tag{4.6}$$

and

$$\rho_{\mathrm{p}}(\boldsymbol{r}) = -\frac{\mathrm{i}e\hbar}{2mc}\boldsymbol{\nabla}\cdot[\psi^\dagger(\boldsymbol{r})\beta\boldsymbol{\alpha}\psi(\boldsymbol{r})]. \tag{4.7}$$

Proceeding analogously, for the unperturbed electronic charge density

$$\rho^{(0)}(\boldsymbol{r}) = -e\psi^{(0)\dagger}(\boldsymbol{r})\psi^{(0)}(\boldsymbol{r}) \tag{4.8}$$

one finds

$$\rho^{(0)}(\boldsymbol{r}) = \rho_{\mathrm{c}}^{(0)}(\boldsymbol{r}) + \rho_{\mathrm{p}}^{(0)}(\boldsymbol{r}), \tag{4.9}$$

with

$$\rho_{\mathrm{c}}^{(0)}(\boldsymbol{r}) = -e\frac{E^{(0)} - V^{(0)}(r)}{mc^2}\psi^{(0)\dagger}(\boldsymbol{r})\beta\psi^{(0)}(\boldsymbol{r}) \tag{4.10}$$

and

$$\rho_{\mathrm{p}}^{(0)}(\boldsymbol{r}) = -\frac{\mathrm{i}e\hbar}{2mc}\nabla\cdot[\psi^{(0)\dagger}(\boldsymbol{r})\beta\boldsymbol{\alpha}\psi^{(0)}(\boldsymbol{r})]. \tag{4.11}$$

Hence, subtracting equation (4.9) from equation (4.5), making use of equation (2.11), and neglecting second- and higher-order terms, we arrive at the following Gordon decomposition of the induced electronic charge density:

$$\rho^{(1)}(\boldsymbol{r}) = \rho_{\mathrm{c}}^{(1)}(\boldsymbol{r}) + \rho_{\mathrm{p}}^{(1)}(\boldsymbol{r}), \tag{4.12}$$

with the convection and spin-polarization components given by

$$\rho_{\mathrm{c}}^{(1)}(\boldsymbol{r}) = -e\frac{E^{(1)} - V^{(1)}(\boldsymbol{r})}{mc^2}\psi^{(0)\dagger}(\boldsymbol{r})\beta\psi^{(0)}(\boldsymbol{r}) - 2e\frac{E^{(0)} - V^{(0)}(r)}{mc^2}\,\mathrm{Re}[\psi^{(0)\dagger}(\boldsymbol{r})\beta\psi^{(1)}(\boldsymbol{r})] \tag{4.13}$$

and

$$\rho_{\mathrm{p}}^{(1)}(\boldsymbol{r}) = \frac{e\hbar}{mc}\mathrm{Im}\nabla\cdot[\psi^{(0)\dagger}(\boldsymbol{r})\beta\boldsymbol{\alpha}\psi^{(1)}(\boldsymbol{r})], \tag{4.14}$$

respectively. Invoking now equation (3.2), we see that the decomposition (4.12) implies the analogous partitioning of the induced electric dipole moment $\boldsymbol{p}^{(1)}$:

$$\boldsymbol{p}^{(1)} = \boldsymbol{p}_{\mathrm{c}}^{(1)} + \boldsymbol{p}_{\mathrm{p}}^{(1)}, \tag{4.15}$$

with

$$\boldsymbol{p}_{\mathrm{c}}^{(1)} = \int_{\mathbb{R}^3}\mathrm{d}^3\boldsymbol{r}\,\boldsymbol{r}\rho_{\mathrm{c}}^{(1)}(\boldsymbol{r}), \qquad \boldsymbol{p}_{\mathrm{p}}^{(1)} = \int_{\mathbb{R}^3}\mathrm{d}^3\boldsymbol{r}\,\boldsymbol{r}\rho_{\mathrm{p}}^{(1)}(\boldsymbol{r}). \tag{4.16}$$

This, in turn, in conjunction with the definition (3.1), gives rise to the Gordon decomposition of the polarizability:

$$\alpha_{\mathrm{d}} = \alpha_{\mathrm{dc}} + \alpha_{\mathrm{dp}}, \tag{4.17}$$

with its convection and spin-polarization parts defined, respectively, by

$$\alpha_{\mathrm{dc}} = \frac{1}{(4\pi\epsilon_0)}\frac{\boldsymbol{F}\cdot\boldsymbol{p}_{\mathrm{c}}^{(1)}}{F^2}, \qquad \alpha_{\mathrm{dp}} = \frac{1}{(4\pi\epsilon_0)}\frac{\boldsymbol{F}\cdot\boldsymbol{p}_{\mathrm{p}}^{(1)}}{F^2}. \tag{4.18}$$

Explicit expressions for α_{dc} and α_{dp} follow from equations (4.18), (4.16), (4.13), (4.14) and (2.20), and from the easily verifiable fact that the first-order energy correction $E^{(1)}$, given by equation (2.15), vanishes. One finds that the convection part of the polarizability has the form

$$\alpha_{\mathrm{dc}} = \alpha_{\mathrm{dc}}' + \alpha_{\mathrm{dc}}'' + \alpha_{\mathrm{dc}}''', \tag{4.19}$$

with the contributions

$$\alpha_{\mathrm{dc}}' = \alpha^2 a_0\int_{\mathbb{R}^3}\mathrm{d}^3\boldsymbol{r}\;\psi^{(0)\dagger}(\boldsymbol{r})\beta(\boldsymbol{n}_z\cdot\boldsymbol{r})^2\psi^{(0)}(\boldsymbol{r}), \tag{4.20}$$

$$\alpha_{\mathrm{dc}}'' = 2\gamma_1\frac{e^2}{(4\pi\epsilon_0)}\mathrm{Re}\int_{\mathbb{R}^3}\mathrm{d}^3\boldsymbol{r}\int_{\mathbb{R}^3}\mathrm{d}^3\boldsymbol{r}'\;\psi^{(0)\dagger}(\boldsymbol{r})\beta\boldsymbol{n}_z\cdot\boldsymbol{r}\mathcal{G}^{(0)}(\boldsymbol{r},\boldsymbol{r}')\boldsymbol{n}_z\cdot\boldsymbol{r}'\psi^{(0)}(\boldsymbol{r}'), \tag{4.21}$$

and

$$\alpha_{\mathrm{dc}}''' = 2\alpha^2 Za_0\frac{e^2}{(4\pi\epsilon_0)}\mathrm{Re}\int_{\mathbb{R}^3}\mathrm{d}^3\boldsymbol{r}\int_{\mathbb{R}^3}\mathrm{d}^3\boldsymbol{r}'\;\psi^{(0)\dagger}(\boldsymbol{r})\beta\boldsymbol{n}_z\cdot\boldsymbol{n}_r\mathcal{G}^{(0)}(\boldsymbol{r},\boldsymbol{r}')\boldsymbol{n}_z\cdot\boldsymbol{r}'\psi^{(0)}(\boldsymbol{r}'). \tag{4.22}$$

The resulting expression for the spin-polarization part of the polarizability,

$$\alpha_{\mathrm{dp}} = -\alpha a_0\frac{e^2}{(4\pi\epsilon_0)}\mathrm{Im}\int_{\mathbb{R}^3}\mathrm{d}^3\boldsymbol{r}\int_{\mathbb{R}^3}\mathrm{d}^3\boldsymbol{r}'\;\boldsymbol{n}_z\cdot\boldsymbol{r}\nabla\cdot[\psi^{(0)\dagger}(\boldsymbol{r})\beta\boldsymbol{\alpha}\mathcal{G}^{(0)}(\boldsymbol{r},\boldsymbol{r}')\boldsymbol{n}_z\cdot\boldsymbol{r}'\psi^{(0)}(\boldsymbol{r}')], \tag{4.23}$$

may be simplified by employing the Gauss divergence theorem and the boundary conditions obeyed by $\psi^{(0)}(\boldsymbol{r})$ and $\mathcal{G}^{(0)}(\boldsymbol{r},\boldsymbol{r}')$ at infinity; one obtains

$$\alpha_{\mathrm{dp}} = \alpha a_0 \frac{e^2}{(4\pi\epsilon_0)} \mathrm{Im} \int_{\mathbb{R}^3} \mathrm{d}^3\boldsymbol{r} \int_{\mathbb{R}^3} \mathrm{d}^3\boldsymbol{r}'\, \psi^{(0)\dagger}(\boldsymbol{r}) \boldsymbol{n}_z \cdot \beta\boldsymbol{\alpha}\mathcal{G}^{(0)}(\boldsymbol{r},\boldsymbol{r}') \boldsymbol{n}_z \cdot \boldsymbol{r}' \psi^{(0)}(\boldsymbol{r}'). \tag{4.24}$$

The angular integration in equation (4.20) may be carried out with the aid of the relation (3.7). One obtains

$$\alpha'_{\mathrm{dc}} = \alpha'_{\mathrm{dc},+1} + \alpha'_{\mathrm{dc},-2}, \tag{4.25}$$

with

$$\alpha'_{\mathrm{dc},+1} = \frac{1}{9}\alpha^2 a_0 \int_0^\infty \mathrm{d}r\, r^2 [P^{(0)}(r)P^{(0)}(r) - Q^{(0)}(r)Q^{(0)}(r)] \tag{4.26}$$

and

$$\alpha'_{\mathrm{dc},-2} = \frac{2}{9}\alpha^2 a_0 \int_0^\infty \mathrm{d}r\, r^2 [P^{(0)}(r)P^{(0)}(r) - Q^{(0)}(r)Q^{(0)}(r)]. \tag{4.27}$$

The radial integral in equations (4.26) and (4.27) is trivial and one finds

$$\alpha'_{\mathrm{dc},+1} = \frac{a_0^3}{Z^4}(\alpha Z)^2 \frac{\gamma_1(\gamma_1+1)(2\gamma_1+1)}{18}, \tag{4.28}$$

$$\alpha'_{\mathrm{dc},-2} = \frac{a_0^3}{Z^4}(\alpha Z)^2 \frac{\gamma_1(\gamma_1+1)(2\gamma_1+1)}{9}. \tag{4.29}$$

In turn, the angular integrals in equations (4.21) and (4.22) may be evaluated with the aid of expansion (3.6) and again formula (3.7). This gives

$$\alpha''_{\mathrm{dc}} = \alpha''_{\mathrm{dc},+1} + \alpha''_{\mathrm{dc},-2}, \qquad \alpha'''_{\mathrm{dc}} = \alpha'''_{\mathrm{dc},+1} + \alpha'''_{\mathrm{dc},-2}, \tag{4.30}$$

with

$$\alpha''_{\mathrm{dc},+1} = \frac{2}{9}\gamma_1 \int_0^\infty \mathrm{d}r \int_0^\infty \mathrm{d}r'\, rr' \begin{pmatrix} P^{(0)}(r) & -Q^{(0)}(r) \end{pmatrix} \mathsf{G}^{(0)}_{+1}(r,r') \begin{pmatrix} P^{(0)}(r') \\ Q^{(0)}(r') \end{pmatrix}, \tag{4.31}$$

$$\alpha''_{\mathrm{dc},-2} = \frac{4}{9}\gamma_1 \int_0^\infty \mathrm{d}r \int_0^\infty \mathrm{d}r'\, rr' \begin{pmatrix} P^{(0)}(r) & -Q^{(0)}(r) \end{pmatrix} \mathsf{G}^{(0)}_{-2}(r,r') \begin{pmatrix} P^{(0)}(r') \\ Q^{(0)}(r') \end{pmatrix}, \tag{4.32}$$

and

$$\alpha'''_{\mathrm{dc},+1} = \frac{2}{9}\alpha^2 Z a_0 \int_0^\infty \mathrm{d}r \int_0^\infty \mathrm{d}r'\, r' \begin{pmatrix} P^{(0)}(r) & -Q^{(0)}(r) \end{pmatrix} \mathsf{G}^{(0)}_{+1}(r,r') \begin{pmatrix} P^{(0)}(r') \\ Q^{(0)}(r') \end{pmatrix}, \tag{4.33}$$

$$\alpha'''_{\mathrm{dc},-2} = \frac{4}{9}\alpha^2 Z a_0 \int_0^\infty \mathrm{d}r \int_0^\infty \mathrm{d}r'\, r' \begin{pmatrix} P^{(0)}(r) & -Q^{(0)}(r) \end{pmatrix} \mathsf{G}^{(0)}_{-2}(r,r') \begin{pmatrix} P^{(0)}(r') \\ Q^{(0)}(r') \end{pmatrix}, \tag{4.34}$$

respectively. The double radial integrals in equations (4.31)–(4.34) may be evaluated with the aid of expansion (3.12) and formula (3.17). After straightforward calculations for $\alpha''_{\mathrm{dc},+1}$ and $\alpha'''_{\mathrm{dc},+1}$, and much more tedious calculations for $\alpha''_{\mathrm{dc},-2}$ and $\alpha'''_{\mathrm{dc},-2}$, exploiting in the latter two cases the Gauss formula (3.19), definition (A.1) and the recurrence relation (3.22), one finds

$$\alpha''_{\mathrm{dc},+1} = \frac{a_0^3}{Z^4} \frac{\gamma_1(\gamma_1+1)(2\gamma_1+1)(2\gamma_1^2+4\gamma_1+3)}{36}, \tag{4.35}$$

$$\alpha''_{\mathrm{dc},-2} = \frac{a_0^3}{Z^4}\left[\frac{\gamma_1^2(\gamma_1+1)(2\gamma_1+1)(2\gamma_1+3)}{9} + \frac{\gamma_1(\gamma_1-2)(2\gamma_1-1)\Gamma^2(\gamma_1+\gamma_2+2)}{18(\gamma_2-\gamma_1+1)\Gamma(2\gamma_1+1)\Gamma(2\gamma_2+1)} \right.$$
$$\left. \times\, {}_3F_2\left(\begin{matrix}\gamma_2-\gamma_1-1,\, \gamma_2-\gamma_1-1,\, \gamma_2-\gamma_1+1 \\ \gamma_2-\gamma_1+2,\, 2\gamma_2+1\end{matrix};1\right)\right], \tag{4.36}$$

$$\alpha'''_{\mathrm{dc},+1} = \frac{a_0^3}{Z^4}(\alpha Z)^2 \frac{(\gamma_1+1)(2\gamma_1+1)}{9}, \tag{4.37}$$

and

$$\alpha'''_{\mathrm{dc},-2} = \frac{a_0^3}{Z^4}(\alpha Z)^2 \left[\frac{(\gamma_1+1)(\gamma_1+2)(2\gamma_1+1)}{9} + \frac{(\gamma_1-2)\Gamma^2(\gamma_1+\gamma_2+2)}{9(\gamma_2-\gamma_1+1)\Gamma(2\gamma_1+1)\Gamma(2\gamma_2+1)} \right.$$
$$\left. \times\, {}_3F_2\left(\begin{matrix} \gamma_2-\gamma_1-1, \gamma_2-\gamma_1-1, \gamma_2-\gamma_1+1 \\ \gamma_2-\gamma_1+2, 2\gamma_2+1 \end{matrix}; 1 \right) \right]. \tag{4.38}$$

Hence, adding expressions (4.28), (4.29) and (4.35)–(4.38), one arrives at the following final form of the convection contribution to the polarizability:

$$\alpha_{\mathrm{dc}} = \frac{a_0^3}{Z^4} \left[\frac{(\gamma_1+1)(2\gamma_1+1)\left(4\gamma_1^2+13\gamma_1+12\right)}{36} - \frac{(\gamma_1-2)^2\Gamma^2(\gamma_1+\gamma_2+2)}{18(\gamma_2-\gamma_1+1)\Gamma(2\gamma_1+1)\Gamma(2\gamma_2+1)} \right.$$
$$\left. \times\, {}_3F_2\left(\begin{matrix} \gamma_2-\gamma_1-1, \gamma_2-\gamma_1-1, \gamma_2-\gamma_1+1 \\ \gamma_2-\gamma_1+2, 2\gamma_2+1 \end{matrix}; 1 \right) \right]. \tag{4.39}$$

Comparison of equation (4.39) with equation (3.24) leads to an unexpected inference: since the right-hand sides of these two equations are identical, the ground-state dipole polarizability of the relativistic hydrogen-like atom is of the purely convective character.

It follows from the remarks concluding the preceding paragraph that the spin-polarization contribution to the polarizability must vanish. Still, it is of interest to ascertain whether α_{dp} vanishes identically or not, i.e., whether all components of α_{dp} due to various angular symmetries vanish or rather an accidental cancellation of some of these components occurs. To resolve this problem, we substitute the expansion (3.6) into equation (4.24) and carrying out angular integrations, one over angles of $\boldsymbol{r}$ with the aid of the known relation

$$\boldsymbol{n}_z \cdot \boldsymbol{\sigma} \Omega_{\kappa m}(\boldsymbol{n}_r) = -\frac{2m}{2\kappa+1}\Omega_{\kappa m}(\boldsymbol{n}_r) - 2\frac{\sqrt{\left(\kappa+\frac{1}{2}\right)^2 - m^2}}{|2\kappa+1|}\Omega_{-\kappa-1,m}(\boldsymbol{n}_r), \tag{4.40}$$

and one over angles of $\boldsymbol{r}'$ with the aid of equation (3.7), we find α_{dp} in the form

$$\alpha_{\mathrm{dp}} = \alpha_{\mathrm{dp},+1} + \alpha_{\mathrm{dp},-2}, \tag{4.41}$$

with

$$\alpha_{\mathrm{dp},+1} = \frac{1}{9}\alpha a_0 \int_0^\infty \mathrm{d}r \int_0^\infty \mathrm{d}r'\, r' \left(Q^{(0)}(r) \quad -3P^{(0)}(r) \right) \mathsf{G}^{(0)}_{+1}(r,r') \begin{pmatrix} P^{(0)}(r') \\ Q^{(0)}(r') \end{pmatrix} \tag{4.42}$$

and

$$\alpha_{\mathrm{dp},-2} = -\frac{4}{9}\alpha a_0 \int_0^\infty \mathrm{d}r \int_0^\infty \mathrm{d}r'\, r' \left(Q^{(0)}(r) \quad 0 \right) \mathsf{G}^{(0)}_{-2}(r,r') \begin{pmatrix} P^{(0)}(r') \\ Q^{(0)}(r') \end{pmatrix}. \tag{4.43}$$

Again, the radial integrals may be carried out by utilizing equations (3.12)–(3.17); hence, one easily obtains

$$\alpha_{\mathrm{dp},+1} = -\frac{a_0^3}{Z^4}(\alpha Z)^2 \frac{(\gamma_1+1)(2\gamma_1+1)}{9} \tag{4.44}$$

and, with some effort,

$$\alpha_{\mathrm{dp},-2} = \frac{a_0^3}{Z^4}(\alpha Z)^2 \frac{(\gamma_1+1)(2\gamma_1+1)}{9}. \tag{4.45}$$

Thus, the total spin-polarization contribution to the polarizablity does indeed vanish:

$$\alpha_{\mathrm{dp}} = 0, \tag{4.46}$$

and this happens because of the accidental cancellation of its two components $\alpha_{\mathrm{dp},+1}$ and $\alpha_{\mathrm{dp},-2}$.

5. Conclusions

In the first part of the paper, using the Sturmian expansion of the generalized first-order Dirac–Coulomb Green function, we have expressed the electric static dipole polarizability of the relativistic hydrogen-like atom in the ground state in terms of a generalized hypergeometric series ${}_3F_2$ of unit argument. The formula derived by us is identical with the one found recently, in a completely different way, by Yakhontov [10] and seems to be the most compact among all known analytical representations of the polarizability [16–22, 11]. In the second part of the paper, we carried out the Gordon decomposition of the polarizability into the convection and spin-polarization parts. Quite unexpectedly, we have found that the spin-polarization part vanishes for all nuclear charges because of an accidental cancellation of its two components.

Appendix A. Some properties of the generalized hypergeometric series ${}_3F_2$ and a derivation of equation (3.22)

The generalized hypergeometric series ${}_3F_2$ is defined as

$$ {}_3F_2\left(\begin{matrix} a_1, a_2, a_3 \\ b_1, b_2 \end{matrix}; z\right) = \frac{\Gamma(b_1)\Gamma(b_2)}{\Gamma(a_1)\Gamma(a_2)\Gamma(a_3)} \sum_{n=0}^{\infty} \frac{\Gamma(a_1+n)\Gamma(a_2+n)\Gamma(a_3+n)}{\Gamma(b_1+n)\Gamma(b_2+n)} \frac{z^n}{n!}. \tag{A.1} $$

In the particular case

$$ b_1 = a_3, \qquad b_2 = b \tag{A.2} $$

it holds

$$ {}_3F_2\left(\begin{matrix} a_1, a_2, a_3 \\ a_3, b \end{matrix}; z\right) = {}_2F_1\left(\begin{matrix} a_1, a_2 \\ b \end{matrix}; z\right), \tag{A.3} $$

where ${}_2F_1$ is the Gauss hypergeometric series.

On exploiting the identity

$$ \frac{1}{\Gamma(b_1+n)} = \frac{1}{(b_1-1)\Gamma(b_1-1+n)} - \frac{n}{(b_1-1)\Gamma(b_1+n)} \tag{A.4} $$

in definition (A.1), one arrives at the recurrence relation

$$ {}_3F_2\left(\begin{matrix} a_1, a_2, a_3 \\ b_1, b_2 \end{matrix}; z\right) = {}_3F_2\left(\begin{matrix} a_1, a_2, a_3 \\ b_1-1, b_2 \end{matrix}; z\right) - \frac{a_1 a_2 a_3 z}{(b_1-1)b_1 b_2} {}_3F_2\left(\begin{matrix} a_1+1, a_2+1, a_3+1 \\ b_1+1, b_2+1 \end{matrix}; z\right). \tag{A.5} $$

Similarly, on using the identity

$$ \frac{1}{\Gamma(a_3+1+n)\Gamma(b+n)} = \frac{1}{b-a_3-1}\left[\frac{1}{\Gamma(a_3+1+n)\Gamma(b-1+n)} - \frac{1}{\Gamma(a_3+n)\Gamma(b+n)}\right], \tag{A.6} $$

from equations (A.1) and (A.3), with the former specialized to the case

$$ b_1 = a_3+1, \qquad b_2 = b, \tag{A.7} $$

one deduces another recurrence relation:

$$ {}_3F_2\left(\begin{matrix} a_1, a_2, a_3 \\ a_3+1, b \end{matrix}; z\right) = \frac{b-1}{b-a_3-1} {}_3F_2\left(\begin{matrix} a_1, a_2, a_3 \\ a_3+1, b-1 \end{matrix}; z\right) - \frac{a_3}{b-a_3-1} {}_2F_1\left(\begin{matrix} a_1, a_2 \\ b \end{matrix}; z\right). \tag{A.8} $$

Setting in equation (A.5)

$$b_1 = a_3 + 1, \qquad b_2 = b - 1 \tag{A.9}$$

and exploiting the result to transform the first term on the right-hand side of equation (A.8), yields

$$\begin{aligned} {}_3F_2\left(\begin{matrix} a_1, a_2, a_3 \\ a_3+1, b \end{matrix}; z\right) &= \frac{b-1}{b-a_3-1}\,{}_2F_1\left(\begin{matrix} a_1, a_2 \\ b-1 \end{matrix}; z\right) - \frac{a_3}{b-a_3-1}\,{}_2F_1\left(\begin{matrix} a_1, a_2 \\ b \end{matrix}; z\right) \\ &\quad - \frac{a_1 a_2 z}{(a_3+1)(b-a_3-1)}\,{}_3F_2\left(\begin{matrix} a_1+1, a_2+1, a_3+1 \\ a_3+2, b \end{matrix}; z\right). \end{aligned} \tag{A.10}$$

In the particular case $z = 1$, after employing the Gauss formula (3.19) and its analogue with b replaced by $b - 1$, equation (A.10) becomes

$$\begin{aligned} {}_3F_2\left(\begin{matrix} a_1, a_2, a_3 \\ a_3+1, b \end{matrix}; 1\right) &= \frac{\Gamma(b)\Gamma(b-a_1-a_2)}{\Gamma(b-a_1)\Gamma(b-a_2)}\left[1 + \frac{a_1 a_2}{(b-a_1-a_2-1)(b-a_3-1)}\right] \\ &\quad - \frac{a_1 a_2}{(a_3+1)(b-a_3-1)}\,{}_3F_2\left(\begin{matrix} a_1+1, a_2+1, a_3+1 \\ a_3+2, b \end{matrix}; 1\right) \\ &\quad (\mathrm{Re}\,(b-a_1-a_2) > 1). \end{aligned} \tag{A.11}$$

This is relation (3.22).

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