Dynamic polarizability of the relativistic hydrogenlike atom: Application of the Sturmian expansion of the Dirac-Coulomb Green function

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We utilize the Sturmian expansion of the Dirac-Coulomb Green function [R. Szmytkowski, J. Phys. B **30**, 825 (1997)] to obtain components of the dynamic dipole polarizability tensor of the relativistic hydrogenlike atom in the ground state. It is found that the tensor may be expressed in terms of two independent quantities: a scalar polarizability and a vector polarizability, the latter being of the relativistic origin. In the static and nonrelativistic limits the previously known expressions for the scalar polarizability are recovered.

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I. INTRODUCTION

A problem of deriving an analytical expression for a scalar dynamic dipole polarizability of a nonrelativistic hydrogenlike atom in a ground state was considered in a number of publications [1–20]. Below a one-photon ionization threshold, with some effort, all available expressions may be transformed to the form

$$\alpha_{\mathrm{s}}(\omega)=\alpha_{\mathrm{s}}^{(+)}(\omega)+\alpha_{\mathrm{s}}^{(-)}(\omega), \tag{1.1}$$

with

$$\alpha_{\mathrm{s}}^{(\pm)}(\omega)=\frac{a_0^3}{Z^4}\frac{2^9(\xi_{\mathrm{nr}}^{(\pm)})^7}{(\xi_{\mathrm{nr}}^{(\pm)}+1)^{12}}\sum_{n=0}^{\infty}\binom{n+3}{n}\times\frac{(n+2-2\xi_{\mathrm{nr}}^{(\pm)})^2}{n+2-\xi_{\mathrm{nr}}^{(\pm)}}\left(\frac{\xi_{\mathrm{nr}}^{(\pm)}-1}{\xi_{\mathrm{nr}}^{(\pm)}+1}\right)^{2n-2}, \tag{1.2}$$

where Z is a nuclear charge (a pointlike and spinless nucleus is assumed), $a_0=\hbar^2/me^2$ is the Bohr radius,

$$\xi_{\mathrm{nr}}^{(\pm)}=\frac{Z}{\lambda_{\mathrm{nr}}^{(\pm)}a_0}, \tag{1.3}$$

and

$$\lambda_{\mathrm{nr}}^{(\pm)}=\sqrt{-\frac{2m(E_{\mathrm{nr}}^{(0)}\pm\hbar\omega)}{\hbar^2}},\quad E_{\mathrm{nr}}^{(0)}=-\frac{Z^2e^2}{2a_0}. \tag{1.4}$$

The representation (1.2) of $\alpha_{\mathrm{s}}^{(\pm)}(\omega)$ is particularly convenient for computational purposes and approximate manipulations. It is most easily obtained by utilizing a Sturmian expansion of the Schrödinger-Coulomb Green function found by Hostler [21].

The validity of the formula (1.2) is restricted to low-Z hydrogenlike atoms. For multiply charged one-electron atoms this expression should be replaced by its counterpart derived within the framework of the relativistic atomic physics based on the Dirac equation. Relativistic formulas for $\alpha_{\mathrm{s}}^{(\pm)}(\omega)$ were obtained by Zapryagaev [22], Florescu *et al.* [23], Pachucki [24,25], and Le Anh Thu *et al.* [26] (who used an oscillator representation of the Dirac-Coulomb Green function). However, Zapryagaev's work is not accessible while the formulas presented in Refs. [23–26] seem not to be direct analogues of Eq. (1.2). It is the purpose of the present paper to derive such an analogue. We obtain also an expression for the vector polarizability of the ground state of a relativistic one-electron atom. In calculations, we make use of the Sturmian expansion of the Dirac-Coulomb Green function constructed by us some time ago [27,28].

II. THE RELATIVISTIC HYDROGENLIKE ATOM IN AN EXTERNAL HARMONICALLY OSCILLATING ELECTRIC FIELD

Consider a hydrogenlike atom with an infinitely heavy pointlike and spinless nucleus of charge $+Ze$ placed in an external homogeneous linearly polarized electric field oscillating harmonically with amplitude $\mathbf{F}$ and frequency ω. The time-dependent Dirac equation describing the dynamics of an atomic electron is

$$\left[-ic\hbar\boldsymbol{\alpha}\cdot\boldsymbol{\nabla}+\beta mc^2-\frac{Ze^2}{r}+e\mathbf{r}\cdot\mathbf{F}\cos(\omega t)-i\hbar\frac{\partial}{\partial t}\right]\Psi(\mathbf{r},t)=0, \tag{2.1}$$

with boundary conditions

$$r\Psi(\mathbf{r},t)\xrightarrow{r\to0}0,\quad r\Psi(\mathbf{r},t)\xrightarrow{r\to\infty}0. \tag{2.2}$$

We shall assume that in the remote past, when the field was being switched on, the atom was in its ground state characterized by the radial quantum number $n=0$, the combined angular momentum and parity quantum number $\kappa=-1$ and the total angular momentum projection quantum number $M=\pm\frac{1}{2}$ (the quantization axis coincides with the direction of $\mathbf{F}$). If the oscillating electric field is weak and causes only a small perturbation of an initial atomic state, we may seek an approximation to an exact solution of the problem (2.1) and (2.2) in the form

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$$\Psi(\mathbf{r},t)\simeq\Psi^{(0)}(\mathbf{r},t)+\Psi^{(1)}(\mathbf{r},t), \tag{2.3}$$

where $\Psi^{(0)}(\mathbf{r},t)$, obeying

$$\left[-ic\hbar\boldsymbol{\alpha}\cdot\boldsymbol{\nabla}+\beta mc^2-\frac{Ze^2}{r}-i\hbar\frac{\partial}{\partial t}\right]\Psi^{(0)}(\mathbf{r},t)=0, \tag{2.4}$$

$$r\Psi^{(0)}(\mathbf{r},t)\xrightarrow{r\to 0}0,\quad r\Psi^{(0)}(\mathbf{r},t)\xrightarrow{r\to\infty}0, \tag{2.5}$$

is the time-dependent wave function of the ground state of the isolated atom. It is given by

$$\Psi^{(0)}(\mathbf{r},t)=\psi^{(0)}(\mathbf{r})\exp(-i\omega^{(0)}t) \tag{2.6}$$

with

$$\psi^{(0)}(\mathbf{r})=\frac{1}{r}\begin{pmatrix}P^{(0)}(r)\Omega_{-1M}(\mathbf{n}_r)\\ iQ^{(0)}(r)\Omega_{+1M}(\mathbf{n}_r)\end{pmatrix}, \tag{2.7}$$

where $\Omega_{\pm\kappa m}(\mathbf{n}_r)$, with $\mathbf{n}_r=\mathbf{r}/r$, are spherical spinors and the radial functions $P^{(0)}(r)$ and $Q^{(0)}(r)$ are

$$P^{(0)}(r)=-\sqrt{\frac{Z}{a_0}\frac{1+\gamma_1}{\Gamma(2\gamma_1+1)}}\left(\frac{2Zr}{a_0}\right)^{\gamma_1}\exp(-Zr/a_0), \tag{2.8}$$

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

Here

$$\hbar\omega^{(0)}=mc^2\gamma_1, \tag{2.10}$$

is the total energy of the ground state of the isolated atom and

$$\gamma_\kappa=\sqrt{\kappa^2-(\alpha Z)^2}, \tag{2.11}$$

where $\alpha=e^2/c\hbar$ (not to be confused with the Dirac vector matrix $\boldsymbol{\alpha}$) denotes the Sommerfeld's fine structure constant.

To find the first-order correction $\Psi^{(1)}(\mathbf{r},t)$, we substitute Eq. (2.3) into the Dirac equation (2.1). Utilizing then Eq. (2.4) and retaining only first-order terms, we find the following differential equation satisfied by $\Psi^{(1)}(\mathbf{r},t)$

$$\left[-ic\hbar\boldsymbol{\alpha}\cdot\boldsymbol{\nabla}+\beta mc^2-\frac{Ze^2}{r}-i\hbar\frac{\partial}{\partial t}\right]\Psi^{(1)}(\mathbf{r},t)=-e\mathbf{r}\cdot\mathbf{F}\Psi^{(0)}(\mathbf{r},t)\cos(\omega t), \tag{2.12}$$

and the appropriate boundary conditions

$$r\Psi^{(1)}(\mathbf{r},t)\xrightarrow{r\to 0}0,\quad r\Psi^{(1)}(\mathbf{r},t)\xrightarrow{r\to\infty}0. \tag{2.13}$$

On utilizing Eq. (2.6), Eq. (2.12) may be equivalently rewritten as

$$\begin{aligned}\left[-ic\hbar\boldsymbol{\alpha}\cdot\boldsymbol{\nabla}+\beta mc^2-\frac{Ze^2}{r}-i\hbar\frac{\partial}{\partial t}\right]\Psi^{(1)}(\mathbf{r},t)\\ =-\frac{1}{2}e\mathbf{r}\cdot\mathbf{F}\psi^{(0)}(\mathbf{r})\exp(-i\omega^{(+)}t)\\ -\frac{1}{2}e\mathbf{r}\cdot\mathbf{F}\psi^{(0)}(\mathbf{r})\exp(-i\omega^{(-)}t),\end{aligned} \tag{2.14}$$

where

$$\omega^{(\pm)}=\omega^{(0)}\pm\omega. \tag{2.15}$$

The particular form of the time-dependence of the right-hand side of Eq. (2.14) suggests that we should seek solutions to this equation in the form

$$\begin{aligned}\Psi^{(1)}(\mathbf{r},t)=\tfrac{1}{2}\psi^{(+)}(\mathbf{r})\exp(-i\omega^{(+)}t)\\ +\tfrac{1}{2}\psi^{(-)}(\mathbf{r})\exp(-i\omega^{(-)}t),\end{aligned} \tag{2.16}$$

where the functions $\psi^{(\pm)}(\mathbf{r})$ satisfy inhomogeneous boundary-value problems

$$\left[-ic\hbar\boldsymbol{\alpha}\cdot\boldsymbol{\nabla}+\beta mc^2-\frac{Ze^2}{r}-E^{(\pm)}\right]\psi^{(\pm)}(\mathbf{r})=-e\mathbf{r}\cdot\mathbf{F}\psi^{(0)}(\mathbf{r}), \tag{2.17}$$

$$r\psi^{(\pm)}(\mathbf{r})\xrightarrow{r\to 0}0,\quad r\psi^{(\pm)}(\mathbf{r})\xrightarrow{r\to\infty}0. \tag{2.18}$$

Provided $E^{(\pm)}=\hbar\omega^{(\pm)}$ do not coincide with any of eigenenergies of the isolated relativistic hydrogenlike atom, time-independent boundary-value problems (2.17) and (2.18) may be solved by using the standard technique of Green functions [29,30]. One finds

$$\psi^{(\pm)}(\mathbf{r})=-e\mathbf{F}\cdot\int_{\mathbb{R}^3}d^3\mathbf{r}'\,\mathcal{G}^{(\pm)}(\mathbf{r},\mathbf{r}')\mathbf{r}'\psi^{(0)}(\mathbf{r}'), \tag{2.19}$$

with

$$\mathcal{G}^{(\pm)}(\mathbf{r},\mathbf{r}')=\mathcal{G}(E^{(\pm)},\mathbf{r},\mathbf{r}'), \tag{2.20}$$

where $\mathcal{G}(E,\mathbf{r},\mathbf{r}')$ is the Dirac-Coulomb Green function satisfying the differential equation

$$\left[-ic\hbar\boldsymbol{\alpha}\cdot\boldsymbol{\nabla}+\beta mc^2-\frac{Ze^2}{r}-E\right]\mathcal{G}(E,\mathbf{r},\mathbf{r}')=\mathcal{I}\delta^{(3)}(\mathbf{r}-\mathbf{r}')\quad[|E|<mc^2], \tag{2.21}$$

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

$$r\mathcal{G}(E,\mathbf{r},\mathbf{r}')\xrightarrow{r\to 0}0,\quad r\mathcal{G}(E,\mathbf{r},\mathbf{r}')\xrightarrow{r\to\infty}0. \tag{2.22}$$

III. THE DYNAMIC POLARIZABILITY TENSOR FOR THE GROUND STATE OF THE RELATIVISTIC HYDROGENLIKE ATOM

The dynamic polarizability tensor $\mathsf{A}(\omega)$ is defined through the relationship

$$\mathbf{p}^{(1)}(t)=\mathrm{Re}\{\mathsf{A}(\omega)\cdot\mathbf{F}\exp(-i\omega t)\}, \tag{3.1}$$

where

$$\mathbf{p}^{(1)}(t)=2\,\mathrm{Re}\int_{\mathbb{R}^3}d^3\mathbf{r}\,\Psi^{(0)\dagger}(\mathbf{r},t)(-e\mathbf{r})\Psi^{(1)}(\mathbf{r},t) \tag{3.2}$$

is an *induced* electric dipole moment of the atom in the perturbed state (2.3). From Eqs. (3.1) and (3.2), on making use of Eqs. (2.6), (2.16), and (2.19), we obtain

$$\mathsf{A}(\omega)=\mathsf{A}^{(+)}(\omega)+\mathsf{A}^{(-)*}(\omega), \tag{3.3}$$

where

$$\mathsf{A}^{(\pm)}(\omega)=e^2\int_{\mathbb{R}^3}d^3\mathbf{r}\int_{\mathbb{R}^3}d^3\mathbf{r}'\,\psi^{(0)\dagger}(\mathbf{r})\mathbf{r}\mathcal{G}^{(\pm)}(\mathbf{r},\mathbf{r}')\mathbf{r}'\,\psi^{(0)}(\mathbf{r}'). \tag{3.4}$$

From now on, we shall work with components of the tensors $\mathsf{A}^{(\pm)}(\omega)$ in a complex spherical basis $\{\mathbf{e}_q\}$, $q=0,\pm1$, orthonormal in the sense of

$$\mathbf{e}_q^*\cdot\mathbf{e}_{q'}=\delta_{qq'}, \tag{3.5}$$

and related to the Cartesian basis $\{\mathbf{n}_Q\}$, $Q=x,y,z$, through

$$\mathbf{e}_q=-\frac{1}{\sqrt{2}}q(\mathbf{n}_x+iq\mathbf{n}_y)+(1-|q|)\mathbf{n}_z. \tag{3.6}$$

With this basis, which, as we shall see soon, is particularly suitable for the present purposes, we have

$$\mathsf{A}^{(\pm)}(\omega)=\sum_{qq'}\alpha_{qq'}^{(\pm)}(\omega)\mathbf{e}_q^*\mathbf{e}_{q'}, \tag{3.7}$$

where

$$\alpha_{qq'}^{(\pm)}(\omega)=e^2\int_{\mathbb{R}^3}d^3\mathbf{r}\int_{\mathbb{R}^3}d^3\mathbf{r}'\,\psi^{(0)\dagger}(\mathbf{r})\times\mathbf{e}_q\cdot\mathbf{r}\mathcal{G}^{(\pm)}(\mathbf{r},\mathbf{r}')\mathbf{e}_{q'}^*\cdot\mathbf{r}'\,\psi^{(0)}(\mathbf{r}'). \tag{3.8}$$

To evaluate the double integral in Eq. (3.8), we shall employ the following Sturmian expansion of the Dirac–Coulomb Green function for $|E|<mc^2$ found in Refs. [27,28]:

$$\mathcal{G}(E,\mathbf{r},\mathbf{r}')=e^{-2}\sum_{n=-\infty}^{\infty}\sum_{\substack{\kappa=-\infty\\(\kappa\neq0)}}^{\infty}\sum_{m=-|\kappa|+1/2}^{|\kappa|-1/2}\frac{1}{\mu_{n\kappa}(\varepsilon)-1}\times\Phi_{n\kappa m}(E,\mathbf{r})\Phi_{n\kappa m}^{\dagger}(E,\mathbf{r}')\mathcal{U}_{n\kappa}(\varepsilon), \tag{3.9}$$

where

$$\mu_{n\kappa}(\varepsilon)=\varepsilon\frac{|n|+\gamma_\kappa+N_{n\kappa}}{\alpha Z}=-\varepsilon\frac{\alpha Z}{|n|+\gamma_\kappa-N_{n\kappa}}, \tag{3.10}$$

and

$$\Phi_{n\kappa m}(E,\mathbf{r})=\frac{1}{r}\begin{pmatrix}S_{n\kappa}(\varepsilon,2\lambda r)\Omega_{\kappa m}(\mathbf{n}_r)\\ \mathrm{i}T_{n\kappa}(\varepsilon,2\lambda r)\Omega_{-\kappa m}(\mathbf{n}_r)\end{pmatrix}, \tag{3.11}$$

with

$$S_{n\kappa}(\varepsilon,2\lambda r)=\sqrt{\frac{\alpha(|n|+2\gamma_\kappa)|n|!}{2\varepsilon N_{n\kappa}(N_{n\kappa}-\kappa)\Gamma(|n|+2\gamma_\kappa)}}\times(2\lambda r)^{\gamma_\kappa}e^{-\lambda r}\left[L_{|n|-1}^{(2\gamma_\kappa)}(2\lambda r)+\frac{\kappa-N_{n\kappa}}{|n|+2\gamma_\kappa}L_{|n|}^{(2\gamma_\kappa)}(2\lambda r)\right], \tag{3.12}$$

$$T_{n\kappa}(\varepsilon,2\lambda r)=\sqrt{\frac{\alpha\varepsilon(|n|+2\gamma_\kappa)|n|!}{2N_{n\kappa}(N_{n\kappa}-\kappa)\Gamma(|n|+2\gamma_\kappa)}}\times(2\lambda r)^{\gamma_\kappa}e^{-\lambda r}\left[L_{|n|-1}^{(2\gamma_\kappa)}(2\lambda r)-\frac{\kappa-N_{n\kappa}}{|n|+2\gamma_\kappa}L_{|n|}^{(2\gamma_\kappa)}(2\lambda r)\right]. \tag{3.13}$$

Here n is a (positive, negative, or zero) integer radial quantum number,

$$N_{n\kappa}=\pm\sqrt{(|n|+\gamma_\kappa)^2+(\alpha Z)^2}=\pm\sqrt{|n|^2+2|n|\gamma_\kappa+\kappa^2} \tag{3.14}$$

is the "apparent principal quantum number" (notice that it may assume positive or negative values),

$$\lambda\equiv\lambda(E)=\frac{\sqrt{(mc^2-E)(mc^2+E)}}{c\hbar}, \tag{3.15}$$

$$\varepsilon\equiv\varepsilon(E)=\sqrt{\frac{mc^2-E}{mc^2+E}}, \tag{3.16}$$

and $\mathcal{U}_{n\kappa}(\varepsilon)$ is a 4×4 matrix defined as

$$\mathcal{U}_{n\kappa}(\varepsilon)=\begin{pmatrix}\mu_{n\kappa}(\varepsilon)I & O\\ O & I\end{pmatrix}, \tag{3.17}$$

where I and O are the 2×2 unit and null matrices, respectively. In Eq. (3.14) the upper sign should be chosen for $n>0$ and the lower one for $n<0$. For $n=0$ one should choose the upper sign if $\kappa<0$ and the lower one if $\kappa>0$.

On substituting the expansion (3.9) to Eq. (3.8) and utilizing Eqs. (2.7) and (3.11), we find

$$\alpha_{qq'}^{(\pm)}(\omega)=\sum_{n\kappa m}d^{1q}(\kappa m,-1M)d^{1q'}(\kappa m,-1M)\frac{I_{n\kappa}^{(\pm)}J_{n\kappa}^{(\pm)}}{\mu_{n\kappa}^{(\pm)}-1}, \tag{3.18}$$

where the real coefficients $d^{kq}(\kappa m,\kappa' m')$ are defined by

$$d^{kq}(\kappa m,\kappa' m') = \sqrt{\frac{4\pi}{2k+1}} \oint_{4\pi} d^2\mathbf{n}_r\, \Omega^{\dagger}_{\kappa' m'}(\mathbf{n}_r) Y_{kq}(\mathbf{n}_r) \Omega_{\kappa m}(\mathbf{n}_r), \tag{3.19}$$

and we have designated

$$\mu_{n\kappa}^{(\pm)} = \mu_{n\kappa}(\varepsilon^{(\pm)}), \tag{3.20}$$

$$I_{n\kappa}^{(\pm)} = \int_0^\infty dr\, r[P^{(0)}(r) S_{n\kappa}^{(\pm)}(r) + Q^{(0)}(r) T_{n\kappa}^{(\pm)}(r)], \tag{3.21}$$

$$J_{n\kappa}^{(\pm)} = \int_0^\infty dr\, r[\mu_{n\kappa}^{(\pm)} P^{(0)}(r) S_{n\kappa}^{(\pm)}(r) + Q^{(0)}(r) T_{n\kappa}^{(\pm)}(r)], \tag{3.22}$$

with

$$S_{n\kappa}^{(\pm)}(r) = S_{n\kappa}(\varepsilon^{(\pm)}, 2\lambda^{(\pm)} r), \tag{3.23}$$

$$T_{n\kappa}^{(\pm)}(r) = T_{n\kappa}(\varepsilon^{(\pm)}, 2\lambda^{(\pm)} r), \tag{3.24}$$

and

$$\lambda^{(\pm)} = \lambda(E^{(\pm)}), \quad \varepsilon^{(\pm)} = \varepsilon(E^{(\pm)}). \tag{3.25}$$

The coefficient (3.19) may be conveniently expressed in terms of Wigner's $3j$ coefficients in the following way:

$$d^{kq}(\kappa m,\kappa' m') = (-1)^{m'+1/2}\sqrt{(2j+1)(2j'+1)} \times \begin{pmatrix} j' & k & j \\ \frac{1}{2} & 0 & -\frac{1}{2} \end{pmatrix} \times \begin{pmatrix} j' & k & j \\ -m' & q & m \end{pmatrix} \pi(l,l',k), \tag{3.26}$$

where

$$\pi(l,l',k) = \begin{cases} 1 & \text{for } l+l'+k \text{ even,} \\ 0 & \text{for } l+l'+k \text{ odd.} \end{cases} \tag{3.27}$$

Deriving Eq. (3.18), we have made use of the symmetry properties

$$(-1)^q d^{k,-q}(\kappa' m',\kappa m) = d^{kq}(\kappa m,\kappa' m'), \tag{3.28}$$

$$d^{kq}(-\kappa m,-\kappa' m') = d^{kq}(\kappa m,\kappa' m'), \tag{3.29}$$

which follow immediately from Eq. (3.26). Due to selection rules obeyed by the Wigner's $3j$ coefficients, we find that

$$\sum_m d^{1q}(\kappa m,-1M) d^{1q'}(\kappa m,-1M) \sim \delta_{qq'}, \tag{3.30}$$

hence, it follows that in the basis chosen the tensors $\mathsf{A}^{(\pm)}(\omega)$ are diagonal. Their elements are

$$\alpha_{qq'}^{(\pm)}(\omega) = [(\tfrac{1}{9}\Delta_{+1}^{(\pm)} + \tfrac{2}{9}\Delta_{-2}^{(\pm)}) + qM(\tfrac{2}{9}\Delta_{+1}^{(\pm)} - \tfrac{2}{9}\Delta_{-2}^{(\pm)})]\delta_{qq'}, \tag{3.31}$$

where

$$\Delta_\kappa^{(\pm)} = \sum_{n=-\infty}^{\infty} \frac{I_{n\kappa}^{(\pm)} J_{n\kappa}^{(\pm)}}{\mu_{n\kappa}^{(\pm)} - 1}. \tag{3.32}$$

Having found components of $\mathsf{A}^{(\pm)}(\omega)$ in the spherical basis, we consider their Cartesian components. Because of the relation (3.6), we have

$$\alpha_{QQ'}^{(\pm)}(\omega) = \alpha_{\mathrm{s}}^{(\pm)}(\omega)\delta_{QQ'} + iM\alpha_{\mathrm{v}}^{(\pm)}(\omega)\varepsilon_{QQ'z}, \tag{3.33}$$

where

$$\alpha_{\mathrm{s}}^{(\pm)}(\omega) = \tfrac{1}{3}\,\mathrm{Tr}\,\mathsf{A}^{(\pm)}(\omega) = \tfrac{1}{9}\Delta_{+1}^{(\pm)} + \tfrac{2}{9}\Delta_{-2}^{(\pm)}, \tag{3.34}$$

$$\alpha_{\mathrm{v}}^{(\pm)}(\omega) = \tfrac{2}{9}\Delta_{+1}^{(\pm)} - \tfrac{2}{9}\Delta_{-2}^{(\pm)}, \tag{3.35}$$

and ε_{ijk} is the Levi-Civita symbol. Hence, for Cartesian components of the dynamic polarizability tensor $\mathsf{A}(\omega)$ we obtain

$$\alpha_{QQ'}(\omega) = \alpha_{\mathrm{s}}(\omega)\delta_{QQ'} + iM\alpha_{\mathrm{v}}(\omega)\varepsilon_{QQ'z}. \tag{3.36}$$

The coefficients

$$\alpha_{\mathrm{s}}(\omega) = \alpha_{\mathrm{s}}^{(+)}(\omega) + \alpha_{\mathrm{s}}^{(-)}(\omega), \tag{3.37}$$

and

$$\alpha_{\mathrm{v}}(\omega) = \alpha_{\mathrm{v}}^{(+)}(\omega) - \alpha_{\mathrm{v}}^{(-)}(\omega), \tag{3.38}$$

are, respectively, the scalar and the vector polarizabilities of the ground state of the one-electron atom.

To proceed further, we have to evaluate the integrals $I_{n\kappa}^{(\pm)}$ and $J_{n\kappa}^{(\pm)}$. On substituting the explicit forms (3.12) and (3.13) of the radial Sturmians to Eqs. (3.21) and (3.22), and performing integrations with the aid of the formula [31]

$$\int_0^\infty dx\, x^\gamma e^{-x/t} L_n^{(\alpha)}(x) = \frac{\Gamma(\gamma+1)\Gamma(\alpha+n+1)}{n!\,\Gamma(\alpha+1)} t^{\gamma+1} {}_2F_1(-n,\gamma+1;\alpha+1;t), \tag{3.39}$$

we obtain

$$I_{n\kappa}^{(\pm)}=\sqrt{\frac{a_0^3}{Z^5}\frac{2^{2\gamma_\kappa+2\gamma_1-1}(\gamma_1+1)\Gamma(|n|+2\gamma_\kappa+1)[\Gamma(\gamma_\kappa+\gamma_1+2)]^2}{\alpha\varepsilon^{(\pm)}|n|!N_{n\kappa}(N_{n\kappa}-\kappa)\Gamma(2\gamma_1+1)[\Gamma(2\gamma_\kappa+1)]^2}}\frac{(\xi^{(\pm)})^{\gamma_1+2}}{(\xi^{(\pm)}+1)^{\gamma_\kappa+\gamma_1+2}}$$
$$\times[|n|[\varepsilon^{(\pm)}(1-\gamma_1)-\alpha Z]F_\kappa^{(\pm)}(-|n|+1)+(N_{n\kappa}-\kappa)[\varepsilon^{(\pm)}(1-\gamma_1)+\alpha Z]F_\kappa^{(\pm)}(-|n|)], \tag{3.40}$$

$$J_{n\kappa}^{(\pm)}=\sqrt{\frac{a_0^3}{Z^5}\frac{\varepsilon^{(\pm)}2^{2\gamma_\kappa+2\gamma_1-1}(\gamma_1+1)\Gamma(|n|+2\gamma_\kappa+1)[\Gamma(\gamma_\kappa+\gamma_1+2)]^2}{\alpha|n|!N_{n\kappa}(N_{n\kappa}-\kappa)\Gamma(2\gamma_1+1)[\Gamma(2\gamma_\kappa+1)]^2}}\frac{(\xi^{(\pm)})^{\gamma_1+2}}{(\xi^{(\pm)}+1)^{\gamma_\kappa+\gamma_1+2}}$$
$$\times[-|n|(N_{n\kappa}+|n|+\gamma_\kappa+\gamma_1-1)F_\kappa^{(\pm)}(-|n|+1)+(N_{n\kappa}-\kappa)(N_{n\kappa}+|n|+\gamma_\kappa-\gamma_1+1)F_\kappa^{(\pm)}(-|n|)], \tag{3.41}$$

where

$$F_\kappa^{(\pm)}(-k)={}_2F_1\left(-k,\gamma_\kappa+\gamma_1+2;2\gamma_\kappa+1;\frac{2}{\xi^{(\pm)}+1}\right), \tag{3.42}$$

and

$$\xi^{(\pm)}=\frac{Z}{\lambda^{(\pm)}a_0}. \tag{3.43}$$

In the case of $\kappa=+1$, Eqs. (3.40) and (3.41) may be simplified if one makes use of the contiguous relation [31]

$$\gamma(\gamma+1)\,{}_2F_1(\alpha,\beta;\gamma;z)=\gamma(\gamma+1)\,{}_2F_1(\alpha,\beta;\gamma+1;z)$$
$$+\alpha\beta z\,{}_2F_1(\alpha+1,\beta+1;\gamma+2;z), \tag{3.44}$$

and the identity [31]

$${}_2F_1(-k,\alpha;\alpha;z)=(1-z)^k \quad [k\in\mathbb{N}]. \tag{3.45}$$

This yields

$$I_{n1}^{(\pm)}=\sqrt{\frac{a_0^3}{Z^5}\frac{2^{4\gamma_1-1}(\gamma_1+1)\Gamma(|n|+2\gamma_1+1)}{\alpha\varepsilon^{(\pm)}|n|!N_{n1}(N_{n1}-1)\Gamma(2\gamma_1+1)}}\frac{(\xi^{(\pm)})^{\gamma_1+2}}{(\xi^{(\pm)}+1)^{2\gamma_1+4}}\left(\frac{\xi^{(\pm)}-1}{\xi^{(\pm)}+1}\right)^{|n|-2}\times\{|n|[\varepsilon^{(\pm)}(1-\gamma_1)-\alpha Z](\xi^{(\pm)}+1)$$
$$\times[(2\gamma_1+1)\xi^{(\pm)}-(2|n|+2\gamma_1-1)]+(N_{n1}-1)[\varepsilon^{(\pm)}(1-\gamma_1)+\alpha Z](\xi^{(\pm)}-1)[(2\gamma_1+1)\xi^{(\pm)}-(2|n|+2\gamma_1+1)]\}, \tag{3.46}$$

$$J_{n1}^{(\pm)}=\sqrt{\frac{a_0^3}{Z^5}\frac{\varepsilon^{(\pm)}2^{4\gamma_1+3}|n|(\gamma_1+1)\Gamma(|n|+2\gamma_1+1)}{\alpha(|n|-1)!N_{n1}(N_{n1}-1)\Gamma(2\gamma_1+1)}}\frac{(\xi^{(\pm)})^{\gamma_1+2}}{(\xi^{(\pm)}+1)^{2\gamma_1+4}}\left(\frac{\xi^{(\pm)}-1}{\xi^{(\pm)}+1}\right)^{|n|-2}$$
$$\times(N_{n1}+|n|+2\gamma_1-1)[|n|+\gamma_1-\xi^{(\pm)}(\gamma_1+1)], \tag{3.47}$$

(notice that $J_{01}^{(\pm)}=0$), hence, collecting terms with the same $|n|$, one arrives at

$$\Delta_{+1}^{(\pm)}=\frac{a_0^3}{Z^4}2^{4\gamma_1+3}(\gamma_1+1)(2\gamma_1+1)\frac{\alpha Z}{\varepsilon^{(\pm)}}\left[1-\left(\frac{\varepsilon^{(\pm)}(1-\gamma_1)}{\alpha Z}\right)^2\right]\frac{(\xi^{(\pm)})^{2\gamma_1+4}}{(\xi^{(\pm)}+1)^{4\gamma_1+8}}$$
$$\times\sum_{n=1}^{\infty}\binom{n+2\gamma_1}{n-1}\frac{[n+\gamma_1-\xi^{(\pm)}(\gamma_1+1)]^2}{n+\gamma_1-\xi^{(\pm)}+\alpha Z\varepsilon^{(\pm)}}\left(\frac{\xi^{(\pm)}-1}{\xi^{(\pm)}+1}\right)^{2n-4}. \tag{3.48}$$

In principle, on collecting terms with the same $|n|$, it is possible to transform the series

$$\Delta_{-2}^{(\pm)}=\sum_{n=-\infty}^{\infty}\frac{I_{n,-2}^{(\pm)}J_{n,-2}^{(\pm)}}{\mu_{n,-2}^{(\pm)}-1}, \tag{3.49}$$

obtained by substituting Eqs. (3.40) and (3.41) with $\kappa=-2$ to Eq. (3.32), to a series in which a summation index runs from 0 to ∞. We do not present the latter series here since, due to a complicated form of its summand, in numerical computations of $\Delta_{-2}^{(\pm)}$ it does not offer any actual advantages over the series (3.49).

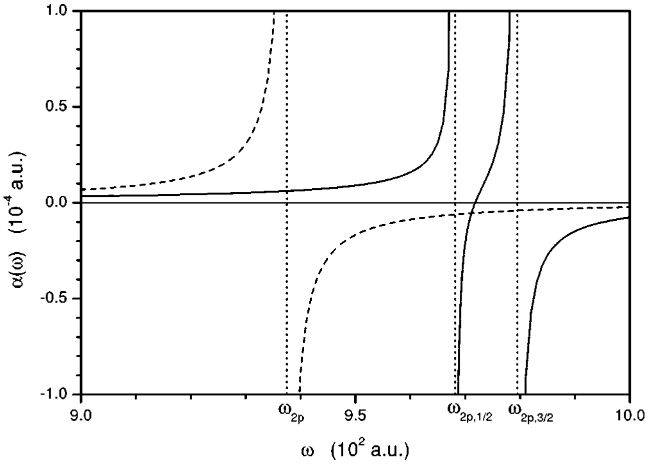

FIG. 1. Plots of relativistic (solid) and nonrelativistic (dashed) scalar dynamic polarizabilities for a one-electron atom of nuclear charge $Z=50$. $\omega_{2\mathrm{p}}$ is a resonant frequency for the nonrelativistic transition $1\mathrm{s}\rightarrow 2\mathrm{p}$ while $\omega_{2\mathrm{p}_{1/2}}$ and $\omega_{2\mathrm{p}_{3/2}}$ are resonant frequencies for the relativistic transitions $1\mathrm{s}_{1/2}\rightarrow 2\mathrm{p}_{1/2}$ and $1\mathrm{s}_{1/2}\rightarrow 2\mathrm{p}_{3/2}$, respectively. Due to the relativistic shift and the fine-structure splitting of energy levels, it holds $\omega_{2\mathrm{p}}<\omega_{2\mathrm{p}_{1/2}}<\omega_{2\mathrm{p}_{3/2}}$.

A plot of the scalar dynamic polarizability for a one-electron atom with $Z=50$ is presented in Fig. 1 in a resonance region corresponding to the transitions $1\mathrm{s}_{1/2}\rightarrow 2\mathrm{p}_{1/2,3/2}$, where relativistic effects are most pronounced. The most distinguished feature of the scalar relativistic polarizability is an additional (compared with the nonrelativistic one) branch located between resonant frequencies $\omega_{2\mathrm{p}_{1/2}}$ and $\omega_{2\mathrm{p}_{3/2}}$.

IV. THE STATIC AND NONRELATIVISTIC LIMITS

A. The static limit

In the static limit $(\omega\rightarrow 0)$ that corresponds to

$$\varepsilon^{(\pm)}\overset{\omega\rightarrow 0}{\rightarrow}\sqrt{\frac{1-\gamma_1}{1+\gamma_1}}=\frac{\alpha Z}{\gamma_1+1},\qquad \xi^{(\pm)}\overset{\omega\rightarrow 0}{\rightarrow}1, \tag{4.1}$$

one easily finds that only the terms with $n=1$ and $n=2$ contribute to the sum on the right of Eq. (3.48) and consequently

$$\Delta_{+1}^{(\pm)}\overset{\omega\rightarrow 0}{\rightarrow}\frac{a_0^3}{Z^4}\frac{\gamma_1(\gamma_1+1)(2\gamma_1+1)(4\gamma_1+5)}{8}, \tag{4.2}$$

that agrees with Eq. (182) of Ref. [27].

In turn, making use of the Gauss relation [31]

$$ {}_2F_1(\alpha,\beta;\gamma;1)=\frac{\Gamma(\gamma)\Gamma(\gamma-\alpha-\beta)}{\Gamma(\gamma-\alpha)\Gamma(\gamma-\beta)}\qquad [\mathrm{Re}(\gamma)>\mathrm{Re}(\alpha+\beta)], \tag{4.3}$$

one finds

$$I_{n,-2}^{(\pm)}\overset{\omega\rightarrow 0}{\rightarrow}\sqrt{\frac{a_0^3}{Z^4}\frac{N_{n,-2}+2}{2^3|n|!N_{n,-2}\Gamma(2\gamma_1+1)\Gamma(|n|+2\gamma_2+1)}}\frac{\Gamma(\gamma_2+\gamma_1+2)\Gamma(|n|+\gamma_2-\gamma_1-2)}{\Gamma(\gamma_2-\gamma_1-1)}\times(-\gamma_1 N_{n,-2}+|n|+\gamma_2+\gamma_1-2), \tag{4.4}$$

$$J_{n,-2}^{(\pm)}\overset{\omega\rightarrow 0}{\rightarrow}\sqrt{\frac{a_0^3}{Z^4}\frac{N_{n,-2}+2}{2^5|n|!N_{n,-2}\Gamma(2\gamma_1+1)\Gamma(|n|+2\gamma_2+1)}}\frac{\Gamma(\gamma_2+\gamma_1+2)\Gamma(|n|+\gamma_2-\gamma_1-2)}{\Gamma(\gamma_2-\gamma_1-1)}\times[(|n|+\gamma_2-\gamma_1-2)(N_{n,-2}+|n|+\gamma_2-\gamma_1+1)-(N_{n,-2}-2)(N_{n,-2}+|n|+\gamma_2+\gamma_1-1)], \tag{4.5}$$

and also

$$\mu_{n,-2}^{(\pm)}\overset{\omega\rightarrow 0}{\rightarrow}\frac{N_{n,-2}+|n|+\gamma_2}{\gamma_1+1}, \tag{4.6}$$

hence, on utilizing Eqs. (4.4) and (4.5) in Eq. (3.49) and collecting terms corresponding to the same $|n|$, one arrives at

$$\Delta_{-2}^{(\pm)}\overset{\omega\rightarrow 0}{\rightarrow}\frac{a_0^3}{Z^4}\frac{1}{2^3\Gamma(2\gamma_1+1)}\left(\frac{\Gamma(\gamma_2+\gamma_1+2)}{\Gamma(\gamma_2-\gamma_1-1)}\right)^2\times\sum_{n=0}^{\infty}\frac{[\Gamma(n+\gamma_2-\gamma_1-2)]^2}{n!(n+\gamma_2-\gamma_1)\Gamma(n+2\gamma_2+1)}f_n(\gamma_1,\gamma_2), \tag{4.7}$$

with

$$f_n(\gamma_1,\gamma_2)=3(1-\gamma_1^2)(n+\gamma_2)^2+(4\gamma_1^3+8\gamma_1^2+\gamma_1-12)\times(n+\gamma_2)-(\gamma_1^4+8\gamma_1^3+\gamma_1^2-12), \quad (4.8)$$

that agrees with Eqs. (183) and (184) of Ref. [27].

Since in the static limit $\Delta_{+1}^{(+)}$ coincides with $\Delta_{+1}^{(-)}$ and $\Delta_{-2}^{(+)}$ coincides with $\Delta_{-2}^{(-)}$, one has $\alpha_{\mathrm{v}}^{(+)}(0)=\alpha_{\mathrm{v}}^{(-)}(0)$. This implies [cf. Eq. (3.38)] that in this limit the vector polarizability $\alpha_{\mathrm{v}}(\omega)$ vanishes, i.e.,

$$\alpha_{\mathrm{v}}(0)=0. \quad (4.9)$$

B. The nonrelativistic limit

In the nonrelativistic limit ($c\to\infty$) one has

$$\gamma_1 \overset{c\to\infty}{\longrightarrow} 1, \quad \gamma_2 \overset{c\to\infty}{\longrightarrow} 2, \quad N_{n,-2} \overset{c\to\infty}{\longrightarrow} \pm(|n|+2), \quad (4.10)$$

$$\xi^{(\pm)} \overset{c\to\infty}{\longrightarrow} \xi_{\mathrm{nr}}^{(\pm)}, \quad \varepsilon^{(\pm)} \overset{c\to\infty}{\longrightarrow} \frac{\alpha Z}{2\xi_{\mathrm{nr}}^{(\pm)}}. \quad (4.11)$$

If $\kappa=+1$, from Eqs. (3.47), (4.10), and (4.11) one obtains

$$\Delta_{+1}^{(\pm)} \overset{c\to\infty}{\longrightarrow} 3\frac{a_0^3}{Z^4}\frac{2^9(\xi_{\mathrm{nr}}^{(\pm)})^7}{(\xi_{\mathrm{nr}}^{(\pm)}+1)^{12}}\sum_{n=1}^{\infty}\binom{n+2}{n-1}\times\frac{(n+1-2\xi_{\mathrm{nr}}^{(\pm)})^2}{n+1-\xi_{\mathrm{nr}}^{(\pm)}}\left(\frac{\xi_{\mathrm{nr}}^{(\pm)}-1}{\xi_{\mathrm{nr}}^{(\pm)}+1}\right)^{2n-4}. \quad (4.12)$$

If $\kappa=-2$, one finds that for $n<0$ it holds

$$J_{n,-2}^{(\pm)} \overset{c\to\infty}{\longrightarrow} 0, \quad (4.13)$$

(and thus the pertinent nonrelativistic limits of $I_{n,-2}^{(\pm)}$ and $\mu_{n,-2}^{(\pm)}$ need not be evaluated), while for $n\geqslant 0$, with the aid of Eq. (3.45), one has

$$I_{n,-2}^{(\pm)} \overset{c\to\infty}{\longrightarrow} -\sqrt{\frac{a_0^3}{Z^4}\frac{2^8(n+3)!}{n!(n+2)}}\frac{(n+2-2\xi_{\mathrm{nr}}^{(\pm)})(\xi_{\mathrm{nr}}^{(\pm)})^{7/2}}{(\xi_{\mathrm{nr}}^{(\pm)}+1)^6}\times\left(\frac{\xi_{\mathrm{nr}}^{(\pm)}-1}{\xi_{\mathrm{nr}}^{(\pm)}+1}\right)^{n-1}, \quad (4.14)$$

$$J_{n,-2}^{(\pm)} \overset{c\to\infty}{\longrightarrow} -\sqrt{\frac{a_0^3}{Z^4}\frac{2^8(n+2)(n+3)!}{n!}}\times\frac{(n+2-2\xi_{\mathrm{nr}}^{(\pm)})(\xi_{\mathrm{nr}}^{(\pm)})^{5/2}}{(\xi_{\mathrm{nr}}^{(\pm)}+1)^6}\left(\frac{\xi_{\mathrm{nr}}^{(\pm)}-1}{\xi_{\mathrm{nr}}^{(\pm)}+1}\right)^{n-1}, \quad (4.15)$$

$$\mu_{n,-2}^{(\pm)} \overset{c\to\infty}{\longrightarrow} \frac{n+2}{\xi_{\mathrm{nr}}^{(\pm)}}, \quad (4.16)$$

that leads to

$$\Delta_{-2}^{(\pm)} \overset{c\to\infty}{\longrightarrow} 3\frac{a_0^3}{Z^4}\frac{2^9(\xi_{\mathrm{nr}}^{(\pm)})^7}{(\xi_{\mathrm{nr}}^{(\pm)}+1)^{12}}\sum_{n=0}^{\infty}\binom{n+3}{n}\times\frac{(n+2-2\xi_{\mathrm{nr}}^{(\pm)})^2}{n+2-\xi_{\mathrm{nr}}^{(\pm)}}\left(\frac{\xi_{\mathrm{nr}}^{(\pm)}-1}{\xi_{\mathrm{nr}}^{(\pm)}+1}\right)^{2n-2}. \quad (4.17)$$

A glance at Eqs. (4.12) and (4.17) shows that in the nonrelativistic limit $\Delta_{+1}^{(\pm)}$ and $\Delta_{-2}^{(\pm)}$ coincide and that, combining these equations with Eq. (3.34), one recovers the nonrelativistic formula (1.2). In addition, one finds

$$\alpha_{\mathrm{v}}(\omega) \overset{c\to\infty}{\longrightarrow} 0. \quad (4.18)$$

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