

Invariant atomic parameters in the ground state of a hydrogenlike atom

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The method of Laplace transformations of the radial Schrödinger equation is used to obtain analytical expressions for the invariant atomic parameters (the dynamical tensor and vector polarizabilities) of a hydrogenlike atom in the ground $1S_{1/2}$ state. These expressions are presented in compact form as linear and quadratic combinations of the hypergeometric functions ${}_2F_1$. The frequency dependence of the invariant atomic parameters is also analyzed. © 1996 American Institute of Physics. [S1063-7761(96)00204-1]

1. INTRODUCTION

The study of the interaction between electromagnetic fields and atoms is an important field of modern atomic physics and spectroscopy. Traditionally the primary role here belongs to the hydrogen atom and hydrogenlike atoms as the simplest quantum systems interacting with an electromagnetic field. In the last decade studies of the behavior of atoms in electromagnetic field have been stimulated by new experimental possibilities opened by the use of high-power lasers in the optical and IR ranges (see the recent papers by Fainstein *et al.*,¹ Manakov *et al.*,² and Damburg *et al.*³ and the literature cited therein). The development of the methods of nonlinear laser spectroscopy⁴ has made it possible to study in experiments not only the fine structure of atomic levels in an external field but also the hyperfine structure.

Manakov and Ovsyannikov⁵ were the first to introduce the concept of invariant atomic parameters to quantitatively describe the excitation of an atomic spectrum by an external monochromatic field. They found that the shift and split of an isolated atomic level produced by a monochromatic laser wave can be expressed in terms of the scalar ($\alpha_s(\omega)$), vector ($\alpha_v(\omega)$), and tensor ($\alpha_t(\omega)$) dynamic polarizabilities of an atom, parameters closely related to the scalar, skew-symmetric, and symmetric Rayleigh scattering of light by an atom. They also found that these parameters are equivalent to the scalar (α_s) and (α_t) polarizabilities of an atom first introduced by Angel and Sandars⁶ for the case of a constant external field.

The polarizability tensor of an atom in an electromagnetic field can be represented in the form of an expansion in irreducible components^{7,8} (here and in what follows summation over repeated indices is implied):

$$\alpha_{ik}(\omega) = \alpha_s(\omega)\delta_{ik} + i\alpha_v(\omega)\varepsilon_{ikn}F_n + \alpha_t(\omega)Q_{ik}, \quad (1)$$

where \mathbf{F} denotes, depending on the nature of the problem, either the total angular momentum of the atom as a whole ($\mathbf{F} = \mathbf{I} + \mathbf{J}$, with \mathbf{I} the nuclear spin and \mathbf{J} the total electron angular momentum) or the atom's total electron angular momentum ($\mathbf{F} = \mathbf{J}$), $Q_{ik} = F_i F_k + F_k F_i - (2/3)F(F+1)\delta_{ik}$, and ω is the frequency of the external monochromatic field. If we ignore the level width, the scalar, vector, and tensor polarizabilities are real-valued and possess the following properties:⁹

$$\alpha_{s,t}(-\omega) = \alpha_{s,t}(\omega), \quad \alpha_v(-\omega) = -\alpha_v(\omega). \quad (2)$$

The scalar polarizability $\alpha_s(\omega)$ in the ground $1S_{1/2}$ state of the hydrogen atom is well-known.¹⁰ The tensor polarizability $\alpha_t(\omega)$ emerges primarily in the ground state only because of the hyperfine coupling between the nucleus and the electron. Its static value ($\omega \rightarrow 0$) was first calculated by Sandars:¹¹ $\alpha_t(0) = -47\alpha^2\mu_N/60$ (atomic units; α is the fine-structure constant, and μ_N is the nuclear magnetic moment in Born-magneton units). The frequency dependence of $\alpha_t(\omega)$ for the ground state of hydrogen was found analytically in Ref. 12. Tensor polarizabilities have also been calculated for the excited states $nS_{1/2}$ and $nP_{1/2}$ of alkali atoms placed in a static field^{13,14} and in a nonresonant light field (for the specific frequencies of neodymium and ruby lasers).⁵

The vector polarizability $\alpha_v(\omega)$ in the ground state of a hydrogenlike atom is caused, as shown by Zhizhimov and Khriplovich,⁸ by relativistic ($\sim \alpha^2$) corrections: first, due to the spin-orbit coupling in highly excited states, and second, due to the presence of an additional contribution to the atomic dipole moment originating in the amplitude of elastic electric dipole scattering of light by the atom, where the amplitude is calculated to within relativistic terms ($\sim v^2/c^2$). The asymptotic frequency dependence of $\alpha_v(\omega)$ for low ω was found by Frantsuzov *et al.*:¹⁵ $\alpha_v(\omega \rightarrow 0) = -(91/72)\alpha^2\omega$. The vector polarizabilities for excited states of alkali atoms were calculated numerically by Manakov and Ovsyannikov⁵ for the frequencies of neodymium and ruby lasers.

In this paper we derive analytical expressions for the vector ($\alpha_v(\omega)$) and tensor ($\alpha_t(\omega)$) dynamic polarizabilities of a hydrogenlike atom in the ground $1S_{1/2}$ state and study their frequency dependence in the entire optical range (far from resonances). We allow for the interaction of the atom with the electric component

$$\mathbf{E}(t) = \mathcal{E} \operatorname{Re}\{e e^{i(\mathbf{kr} - \omega t)}\} \quad (e e^* = 1) \quad (3)$$

of the laser wave (the electric dipole approximation) but ignore the magnetic component and the spatial inhomogeneity of the field.² In Secs. 2 and 3, we derive closed compact analytical expressions for, respectively, the tensor ($\alpha_t(\omega)$) and vector ($\alpha_v(\omega)$) dynamic polarizabilities in the ground

$1S_{1/2}$ state of a hydrogenlike atom. Section 4 discusses the results of the two preceding sections. Throughout the article we use the Coulomb system of units.

2. DYNAMIC TENSOR POLARIZABILITY

Since the total electron angular momentum in the $1S_{1/2}$ state is $J=1/2$, the tensor polarizability in this state can arise only because of hyperfine electron–nucleus coupling.¹¹ The corresponding Schrödinger equation in the atom's center-of-mass system has the form

$$\left(-\frac{1}{2}\Delta - \frac{1}{r} + \hat{H}_{\text{hf}} + \hat{H}_E(t)\right)\Psi(\mathbf{r},t) = i\frac{\partial}{\partial t}\Psi(\mathbf{r},t), \quad (4)$$

where

$$\hat{H}_{\text{hf}} = \frac{\alpha^2 \mu_N}{2I} \left(\frac{8\pi}{3} \mathbf{I} \cdot \mathbf{S} \delta(\mathbf{r}) - \frac{\sqrt{10}}{r^3} \mathbf{I} \cdot \{C^2(\mathbf{n} \cdot \mathbf{S})\}^1 \right) - \frac{C^2(\mathbf{n}) \cdot Q^2}{r^3}$$

is the operator of the hyperfine electron–nucleus coupling¹⁶ ($\mathbf{n}=\mathbf{r}/r$), and

$$\hat{H}_E(t) = k_1 \hat{Z} \mathcal{E} \cos(\omega t), \quad k_1 = \frac{m_N + Z}{m_N + 1},$$

is the electric dipole interaction of the atom and the laser wave (3). In this section the wave is assumed plane-polarized, and the quantization axis \mathbf{Z} is directed along the wave's polarization vector. The mass factor k_1 appears because of the transition to the atom's center-of-mass system¹⁷ and will be discarded.

We use the following notation in Eq. (4): α is the fine-structure constant, \mathbf{I} and \mathbf{S} are the nuclear and electron spin operators, μ_N is the nuclear magnetic moment expressed in Born-magneton units, Q^2 is the nuclear quadruple-moment tensor, $C_m^2(\mathbf{n}) = \sqrt{4\pi/5} Y_{2m}(\mathbf{n})$ is the modified spherical harmonic of rank 2, and $A \cdot B$ and $\{A \cdot B\}^p$ stand for the scalar (or rank p) products of the operators A and B .

As is well known, the z -component of the atomic dipole moment induced by an external field is¹⁸

$$d_z^{\text{(ind)}}(t) = \alpha_{zz}(\omega) \mathcal{E} \cos(\omega t), \quad (5)$$

where $\alpha_{zz}(\omega)$ is the zz -component of the polarizability tensor (1). To simplify matters we assume that the component is taken in the $1S_{1/2}$ state of the atom with the maximum projection of total angular momentum \mathbf{F} . Note that in our problem the total spin $\mathbf{I} + \mathbf{S}$ and the projection of the total angular momentum on the quantization axis are conserved, while the total angular momentum is not conserved because of the mixing of states with orbital angular momenta $l \neq 0$ and the ground state. Such mixing is caused by the operators of the hyperfine and electric dipole interactions.

On the other hand, $d_z^{\text{(ind)}}$ is determined by the average value of the atomic dipole moment operator:

$$d_z^{\text{(ind)}}(t) = -\langle \Psi(\mathbf{r},t) | \hat{Z} | \Psi(\mathbf{r},t) \rangle, \quad (6)$$

where the wave function $\Psi(\mathbf{r},t)$ is calculated from Eq. (4) in second-order perturbation theory in the operators of hyperfine and electric dipole interaction:

$$\Psi(\mathbf{r},t) = \Psi^{(0)} + \Psi_E^{(1)} + \Psi_{\text{hf}}^{(1)} + \Psi_{\text{hf},E}^{(2)} + \Psi_E^{(2)} + \Psi_{\text{hf}}^{(2)}.$$

Here

$$\Psi^{(0)}(\mathbf{r},t) = \frac{1}{\sqrt{\pi}} \exp(-iE^{(0)}t) \exp(-r) \chi_{FF}$$

is the unperturbed wave function of a hydrogenlike atom in the ground $1S_{1/2}$ state with the maximum projection of the total angular momentum (actually the total spin, since for S states the values of total angular momentum and total spin coincide), $E^{(0)} = -1/2$ is the unperturbed ground-state energy, and χ_{FF} is the spin part of the wave function corresponding to the total spin $\mathbf{I} + \mathbf{S} = \mathbf{F}$ and its maximum projection on the quantization axis equal to F . The corrections to $\Psi^{(0)}(\mathbf{r},t)$ are caused by the electric dipole interaction, the hyperfine coupling, and their combined action.

Comparing (5) and (6) and allowing for (1), we arrive at the following expression for the dynamic tensor polarizability of a hydrogenlike atom in the ground state:

$$\alpha_t(\omega) \mathcal{E} \cos(\omega t) = -\frac{3}{2F(2F-1)} \text{Re} \{ \langle \Psi^{(0)} \times (\mathbf{r},t) | \hat{Z} | \Psi_{\text{hf},E}^{(2)}(\mathbf{r},t) \rangle + \langle \Psi_E^{(1)} \times (\mathbf{r},t) | \hat{Z} | \Psi_{\text{hf}}^{(1)}(\mathbf{r},t) \rangle \}. \quad (7)$$

According to (7), to calculate $\alpha_t(\omega)$ we must know the corrections $\Psi_E^{(1)}$, $\Psi_{\text{hf}}^{(1)}$, and $\Psi_{\text{hf},E}^{(2)}$ to the unperturbed wave function. Here the terms $\Psi_{\text{hf}}^{(1)}$ and $\Psi_{\text{hf},E}^{(2)}$, caused by the contact part of the hyperfine coupling in (4), can, obviously, contribute only to the scalar polarizability and therefore will be ignored. Below we always interpret $\Psi_{\text{hf}}^{(1)}$ and $\Psi_{\text{hf},E}^{(2)}$ as functions caused by the noncentral part of H_{hf} .

Schwartz¹⁹ was the first to calculate $\Psi_{\text{hf}}^{(1)}(\mathbf{r},t)$ for the hydrogen atom. It is convenient to write this correction for a hydrogenlike atom with an arbitrary nuclear spin as

$$\Psi_{\text{hf}}^{(1)}(\mathbf{r},t) = (\alpha^2 \mu_N \eta_F^{\mu} + Q \eta_F^Q) \exp(-iE^{(0)}t) \frac{1}{3r} \times \left(1 + \frac{r}{3} \right) e^{-r} (Y_2(\mathbf{n}) \otimes \chi_F)^{FF}, \quad (8)$$

where

$$\eta_F^{\mu} = -3 \sqrt{\frac{(2F+1)(I+1)(2I+1)}{I}} \begin{Bmatrix} F & F & 2 \\ I & I & 1 \\ 1/2 & 1/2 & 1 \end{Bmatrix},$$

$$\eta_F^Q = 2(-1)^{1/2+I+F} \sqrt{\frac{(2F+1)(I+1)(2I+1)(2I+3)}{5I(2I-1)}} \times \begin{Bmatrix} 2 & I & I \\ 1/2 & F & F \end{Bmatrix} \quad (8a)$$

are the spin factor originating, respectively, in the magnetic dipole–dipole and quadruple parts of the hyperfine coupling operator in (4), Q is the quadruple moment of the nucleus,

⊗ stands for the direct product of the spherical harmonic $Y_2(\mathbf{n})$ and the spin function χ_F , and $F = I \pm 1/2$.

The correction functions $\Psi_E^{(1)}$ and $\Psi_{\text{hf},E}^{(2)}(\mathbf{r},t)$ can be found by solving the appropriate perturbation-theory equations obtained from the initial equation (4). A detailed description of the procedure for calculating these functions by the method of Laplace transformations^{20,21} for the simplest case of atomic hydrogen can be found in Ref. 12. For a hydrogenlike atom with an arbitrary nuclear spin, the fact that the spin structure of the noncentral part of the hyperfine coupling in (4) is more complicated and the presence of an additional quadruple term lead to an additional spin dependence of the Laplace transforms of the radial parts of the corrections $\Psi_E^{(1)}$ and $\Psi_{\text{hf},E}^{(2)}$. Leaving out the intermediate calculations (see Ref. 12), we give only the final expressions. The correction $\Psi_E^{(1)}$ has the form

$$\begin{aligned} \Psi_E^{(1)}(\mathbf{r},t) &= u_{(+)}(\mathbf{r},\omega) \exp[-i(E^{(0)} + \omega)t] + u_{(-)}(\mathbf{r},\omega) \exp[-i(E^{(0)} - \omega)t], \\ u_{(\pm)}(\mathbf{r},t) &= \sum_{F'=F}^{F+1} r^2 \varphi_{F'}^{(\pm)}(r,\omega) (Y_1(\mathbf{n}) \otimes \chi_F)^{F'F}. \end{aligned} \quad (9)$$

We can write the Laplace transforms of the radial functions $\varphi_{F',F+1}^{(\pm)}(r,\omega)$ in terms of linear combinations of Gauss's hypergeometric functions ${}_2F_1$ (see Ref. 22):

$$\begin{aligned} F_{F',F+1}^{(\pm)}(p,\omega) &= \int_0^\infty dr e^{-pr} \varphi_{F',F+1}^{(\pm)}(r,\omega) = \eta_{F',F+1}^E \\ &\times \Phi^{(\pm)}(p,\omega) = \eta_{F',F+1}^E \\ &\times \frac{3 \times 2^6 \kappa^3}{(1+\kappa)^5} \left\{ {}_2F_1 \left(5, 2 - \frac{1}{\kappa}, 3 \right. \right. \\ &\left. \left. - \frac{1}{\kappa}, \frac{(1-\kappa)(p-\kappa)}{(1+\kappa)(p+\kappa)} \right) \right. \\ &\times \frac{1}{(2-1/\kappa)(p+\kappa)^4} - {}_2F_1 \left(5, 3 - \frac{1}{\kappa}, 4 \right. \\ &\left. \left. - \frac{1}{\kappa}, \frac{(1-\kappa)(p-\kappa)}{(1+\kappa)(p+\kappa)} \right) \frac{p-\kappa}{(3-1/\kappa)(p+\kappa)^5} \right\}, \end{aligned} \quad (10)$$

where $\kappa = \sqrt{1+2\omega}$, $\Phi^{(\pm)}(p,\omega)$ is a function which does not depend on the spin variables, and $\eta_F^E = (4/\sqrt{3}) C_{FF10}^{FF}$ and $\eta_{F+1}^E = -(1/\sqrt{F}) \eta_F^E$ are spin factors dependent on the angular part of the electric dipole interaction in (4), where C_{FF10}^{FF} is a Clebsch-Gordan coefficient.

The correction $\Phi_{\text{hf},E}^{(2)}(\mathbf{r},t)$ is given by similar expressions:

$$\begin{aligned} \Psi_{\text{hf},E}^{(2)}(\mathbf{r},t) &= u_{(+)}(\mathbf{r},\omega) \exp[-i(E^{(0)} + \omega)t] \\ &\quad + v_{(-)}(\mathbf{r},\omega) \exp[-i(E^{(0)} - \omega)t], \\ u_{(\pm)}(\mathbf{r},t) &= \sum_{F'=F}^{F+1} r^2 h_{F'}^{(\pm)}(r,\omega) (Y_1(\mathbf{n}) \otimes \chi_F)^{F'F}. \end{aligned} \quad (11)$$

We can write the Laplace transforms of the radial functions $h_{F',F+1}^{(\pm)}(r,\omega)$ as follows:

$$\begin{aligned} H_{F',F+1}^{(\pm)}(p,\omega) &= \lambda_{F',F+1} (\alpha^2 \mu_N \eta_F^\mu + Q \eta_F^Q) D^{(\pm)}(p,\omega) \\ &= \lambda_{F',F+1} (\alpha^2 \mu_N \eta_F^\mu \\ &\quad + Q \eta_F^Q) \frac{2^6 \sqrt{3} \kappa^3}{9(1+\kappa)^5} \left\{ {}_2F_1 \left(4, 2 - \frac{1}{\kappa}, 3 \right. \right. \\ &\quad \left. \left. - \frac{1}{\kappa}, \frac{(1-\kappa)(p-\kappa)}{(1+\kappa)(p+\kappa)} \right) \frac{3(1+\kappa)}{4(2-1/\kappa)(p+\kappa)^4} \right. \\ &\quad \left. + {}_2F_1 \left(5, 2 - \frac{1}{\kappa}, 3 - \frac{1}{\kappa}, \frac{(1-\kappa)(p-\kappa)}{(1+\kappa)(p+k)} \right) \right. \\ &\quad \times \frac{1}{(2-1/\kappa)(p+\kappa)^4} - {}_2F_1 \left(5, 3 - \frac{1}{\kappa}, 4 \right. \\ &\quad \left. \left. - \frac{1}{\kappa}, \frac{(1-\kappa)(p-\kappa)}{(1+\kappa)(p+k)} \right) \right. \\ &\quad \times \frac{p-\kappa}{(3-1/\kappa)(p+\kappa)^5} - \frac{2}{\sqrt{3}(p^2-\kappa^2)^2} \\ &\quad \times \left(\frac{p-\kappa}{p+\kappa} \right)^{1/\kappa} \int_\kappa^p dt (t^2 - \kappa^2) \\ &\quad \left. \times \left(\frac{t+\kappa}{t-\kappa} \right)^{1/\kappa} \int_t^\infty dt' \int_{t'}^\infty dt'' \Phi^{(\pm)}(t'',\omega) \right\}, \end{aligned} \quad (12)$$

where $D^{(\pm)}(p,\omega)$ is a function that does not depend on the spin variables, and

$$\lambda_F = (-1)^{2F+1} 2 \sqrt{6(2F+1)} C_{FF10}^{FF} \begin{Bmatrix} F & F & 2 \\ 1 & 1 & F \end{Bmatrix},$$

$$\lambda_{F+1} = \frac{\sqrt{F}}{2F+3} \lambda_F$$

are the spin factors originating in the hyperfine and electric dipole interactions. Selecting $p = \kappa$ as the lower limit in an integral in (12) guarantees that the functions $H_{F',F+1}^{(\pm)}(p,\omega)$ behave at this point as analytic functions, which corresponds to the correct behavior of the radial functions $h_{F',F+1}^{(\pm)}(r,\omega)$ at infinity and is sufficient for finding a unique solution.²³

The calculation of the dynamic tensor polarizability (7) is reduced to integrating the radial functions $\varphi_{F',F+1}^{(\pm)}(r,\omega)$ and $h_{F',F+1}^{(\pm)}(r,\omega)$. This in turn can be reduced to finding the derivatives of the corresponding Laplace transforms $F_{F',F+1}^{(\pm)}(p,\omega)$ and $H_{F',F+1}^{(\pm)}(p,\omega)$ with respect to the Laplace variable according to the following scheme:

$$\int_0^\infty dr f(r,\omega) r^n e^{-r} = (-1)^n \frac{d^n}{dp^n} F(p,\omega) \Big|_{p=1}, \quad (13)$$

$$F(p,\omega) = \int_0^\infty dr f(r,\omega) e^{-pr}.$$

As a result the polarizability (7), written in terms of Laplace variables, assumes the form

$$\alpha_i(\omega) = \alpha(+\omega) + \alpha(-\omega), \quad (14)$$

$$\alpha(\pm\omega) = -\frac{3(F+1)}{2F(2F+3)(2F-1)}\eta_F^E\lambda_F(\alpha^2\mu_N\eta_F^\mu + Q\eta_F^Q)\left\{\frac{d}{dp}D^{(\pm)}(p,\omega) + \frac{1}{3\sqrt{3}}\left(\Phi^{(\pm)}(p,\omega) - \frac{1}{3}\frac{d}{dp}\Phi^{(\pm)}(p,\omega)\right)\right\}\Big|_{p=1},$$

where the functions $\Phi^{(\pm)}(p,\omega)$ and $D^{(\pm)}(p,\omega)$ are specified by (10) and (12), respectively.

After simplifying Eq. (14) by using the properties of hypergeometric functions²² and employing Eqs. (10) and (12), we arrive at the following analytical expression for the dynamic tensor polarizability of a hydrogenlike atom in the ground $^1S_{1/2}$ state:

$$\alpha_t(\omega) = K(F)[\beta(+\omega) + \beta(-\omega)], \quad (15)$$

$$\begin{aligned} \beta(\pm\omega) = & -\frac{4}{15\kappa(1+\kappa)} - \frac{2^{10}\kappa^3}{15(1+\kappa)^{11}(2\kappa-1)(3\kappa-1)} \left\{ (24\kappa^4 + 49\kappa^3 + 17\kappa^2 - 9\kappa - 1) {}_2F_1\left(5, 2 - \frac{1}{\kappa}, 3 - \frac{1}{\kappa}, \left(\frac{1-\kappa}{1+\kappa}\right)^2\right) + (12\kappa^4 - 4\kappa^3 - 21\kappa^2 + 8\kappa + 1) {}_2F_1\left(5, 3 - \frac{1}{\kappa}, 4 - \frac{1}{\kappa}, \left(\frac{1-\kappa}{1+\kappa}\right)^2\right) + A(\kappa) \right. \\ & \times \left[(3\kappa-1)(6\kappa-1)\left(1 + \frac{1}{\kappa}\right)^2 - 2 {}_2F_1\left(2, 3 - \frac{1}{\kappa}, 4 - \frac{1}{\kappa}, \frac{1-\kappa}{1+\kappa}\right) \right] + 2\kappa \sum_{\substack{n=2 \\ (n \neq 4)}}^6 B_n(\kappa) \\ & \times \left[{}_2F_1\left(n, 3 - \frac{1}{\kappa}, 4 - \frac{1}{\kappa}, \frac{1-\kappa}{1+\kappa}\right) \right. \\ & \left. \left. \times \frac{n-1}{(3\kappa-1)(1+\kappa)} - \frac{4}{1+\kappa} \left(\frac{1+\kappa}{2\kappa}\right)^n \right] \right\}, \end{aligned}$$

where

$$K(F) = -\frac{1}{4}\sqrt{\frac{5}{F(F+1)(2F+3)(2F-1)}}(\alpha^2\mu_N\eta_F^\mu + Q\eta_F^Q), \quad F=I+\frac{1}{2}, \quad \kappa = \sqrt{1+2\omega},$$

$$\begin{aligned} A(\kappa) = & 3\kappa^2 \left\{ {}_2F_1\left(5, 2 - \frac{1}{\kappa}, 3 - \frac{1}{\kappa}, \frac{1-\kappa}{1+\kappa}\right) \frac{1}{2\kappa-1} - {}_2F_1\left(5, 3 - \frac{1}{\kappa}, 4 - \frac{1}{\kappa}, \frac{1-\kappa}{1+\kappa}\right) \frac{1}{3\kappa-1} \right\}, \\ B_2(\kappa) = & 15\kappa^3 \left(\frac{1-\kappa}{1+\kappa}\right) \left\{ {}_2F_1\left(6, 4 - \frac{1}{\kappa}, 5 - \frac{1}{\kappa}, \frac{\kappa-1}{\kappa+1}\right) \frac{2\kappa}{4\kappa-1} + (6\kappa - 4) {}_2F_1\left(6, 1, 2, \frac{\kappa-1}{\kappa+1}\right) \right\}, \quad (15a) \end{aligned}$$

$$\begin{aligned} B_3(\kappa) = & \frac{30\kappa^3}{2\kappa-1} \left(\frac{1-\kappa}{1+\kappa}\right) \left\{ - {}_2F_1\left(6, 4 - \frac{1}{\kappa}, 5 - \frac{1}{\kappa}, \frac{\kappa-1}{\kappa+1}\right) \frac{2\kappa^2}{4\kappa-1} + 3(5\kappa^2 - 4\kappa + 1) {}_2F_1\left(6, 1, 2, \frac{\kappa-1}{\kappa+1}\right) - (3\kappa-1)(\kappa+1) \right. \\ & \left. \times \left(\frac{\kappa+1}{2}\right)^5 \right\}, \end{aligned}$$

$$\begin{aligned} B_5(\kappa) = & -\frac{360\kappa^3}{(2\kappa-1)(1+\kappa)} \left\{ {}_2F_1\left(6, 4 - \frac{1}{\kappa}, 5 - \frac{1}{\kappa}, \frac{\kappa-1}{\kappa+1}\right) \frac{2\kappa^4}{4\kappa-1} + \frac{33\kappa^5 - 63\kappa^4 + 75\kappa^3 - 51\kappa^2 + 16\kappa - 2}{6(\kappa-1)^2} {}_2F_1\left(6, 1, 2, \frac{\kappa-1}{\kappa+1}\right) \right. \\ & \left. - \frac{(3\kappa-1)(3\kappa^4 + \kappa^2 + 2\kappa - 2)}{6(\kappa-1)^2} \left(\frac{\kappa+1}{2}\right)^5 \right\}, \end{aligned}$$

$$\begin{aligned} B_6(\kappa) = & -\frac{1800\kappa^3}{(2\kappa-1)(1+\kappa)^2} \left\{ {}_2F_1\left(6, 4 - \frac{1}{\kappa}, 5 - \frac{1}{\kappa}, \frac{\kappa-1}{\kappa+1}\right) \frac{2\kappa^5}{4\kappa-1} + \frac{\kappa(5\kappa^5 + 2\kappa^4 + 3\kappa^3 + \kappa^2 - 4\kappa + 1)}{2(\kappa-1)^2} {}_2F_1\left(6, 1, 2, \frac{\kappa-1}{\kappa+1}\right) \right. \\ & \left. - \frac{(3\kappa-1)(9\kappa^5 + 9\kappa^4 + 20\kappa^3 + 31\kappa^2 + 7\kappa - 16)}{30(\kappa-1)^2} \right. \\ & \left. \times \left(\frac{\kappa+1}{2}\right)^5 \right\}. \end{aligned}$$

3. VECTOR POLARIZABILITY

Zhizhimov and Khriplovich⁸ were the first to point out that vector polarizability is present in the ground state of hydrogen (or a hydrogenlike atom). According to them, such polarizability emerges, first, because of spin-orbit splitting of excited levels and, second, because of a relativistic correction ($\sim \alpha^2$) to the operator of the atom's dipole moment. The spin-orbit splitting of excited levels is caused by the spin-orbit coupling¹⁸

$$\hat{W} = \frac{\alpha^2}{2r^3} \mathbf{L} \mathbf{S} \quad (16)$$

(here, as usual, \mathbf{L} is the operator of the electron's orbital angular momentum, and \mathbf{S} is the electron spin operator) in states with $l \neq 0$. The correction to the dipole moment operator emerges as a consequence of a formal mathematic device that makes it possible to avoid calculating relativistic corrections to the wave functions in computations of the amplitude $f^{E1, E1}$ of elastic electric dipole scattering of light by an atom within terms of order v^2/c^2 . Instead, as shown in Ref. 8, one can use nonrelativistic wave functions, redefining, however, the atom's electric dipole moment:

$$\mathbf{d} = -\mathbf{r} - \frac{1}{2} \alpha^2 \mathbf{p} \times \mathbf{S}, \quad (17)$$

where \mathbf{p} is the momentum of an outer-shell electron in the atom.

The expression for the vector polarizability in the ground state of a hydrogenlike atom, as that for the tensor polarizability, can be obtained by calculating the induced dipole moment of the atom in a state with the wave function

$$\begin{aligned} \Psi(\mathbf{r}, t) = & \Psi^{(0)} + \Psi_E^{(1)} + \alpha^2 \bar{\Psi}_E^{(1)} + \Psi_E^{(2)} + \alpha^4 \bar{\Psi}_E^{(2)} \\ & + \alpha^2 \Psi_{W,E}^{(2)} + \alpha^4 \bar{\Psi}_{W,E}^{(2)}, \end{aligned} \quad (18)$$

where

$$\Psi^{(0)}(\mathbf{r}, t) = \frac{1}{\sqrt{\pi}} \exp(-iE^{(0)}t) \exp(-r) \chi_{1/2m}$$

is the unperturbed wave function of the ground level $1S_{1/2}$ (without allowing for the hyperfine structure), and $\chi_{1/2m}$ is the spin part of the function. The corrections $\Psi_E^{(i)}$ ($i=1,2$) and $\Psi_{W,E}^{(2)}$ to the unperturbed wave function are caused, respectively, by the electric dipole interaction (without the relativistic correction) and by the combination of this interaction and the spin-orbit coupling (16). The functions $\bar{\Psi}_E^{(i)}$ ($i=1,2$) and $\bar{\Psi}_{W,E}^{(2)}$ are similar corrections caused, however, by the relativistic term ($\sim \alpha^2$) in the dipole moment operator (17). In (18) we have allowed for the fact that the functions $\Psi_W^{(i)}$ ($i=1,2$) are identically zero for the S states of the atom.

Averaging the dipole moment operator (17) over the state (18) with allowance for (1) and (3), we arrive at the following expression for the vector polarizability:

$$\begin{aligned} i\alpha_v(\omega) \varepsilon_{ikn} J_k \mathcal{E} \operatorname{Re}\{\mathbf{e}_n e^{-i\omega t}\} = & -2\alpha^2 \operatorname{Re}\{2\langle \Psi^{(0)} | \\ & \times (\mathbf{r}, t) | \frac{1}{2} [\mathbf{p} \mathbf{S}]_i | \Psi_E^{(1)}(\mathbf{r}, t) \rangle + \langle \Psi^{(0)}(\mathbf{r}, t) | \mathbf{r}_i | \Psi_{W,E}^{(2)} \\ & \times (\mathbf{r}, t) \rangle\}. \end{aligned} \quad (19)$$

where \mathbf{J} is the total electron angular momentum of the atom, and the electromagnetic wave (3) is assumed circularly polarized.

In calculating $\alpha_v(\omega)$ one can use the results of Sec. 2. By analogy with (9), the first-order correction $\Psi_E^{(1)}(\mathbf{r}, t)$ has the form

$$\begin{aligned} \Psi_E^{(1)}(\mathbf{r}, t) = & u_{(+)}(\mathbf{r}, \omega) \exp[-i(E^{(0)} + \omega)t] + u_{(-)} \\ & \times (\mathbf{r}, \omega) \exp[-i(E^{(0)} - \omega)t], \end{aligned} \quad (20)$$

$$u_{(\pm)}(\mathbf{r}, \omega) = \sum_{J=1/2}^{3/2} r^2 \varphi_J^{(\pm)}(r, \omega) (Y_1(\mathbf{n}) \otimes \chi_{1/2})^{Jm_J}.$$

Such notation corresponds to the case where the hyperfine structure is ignored in comparison to the fine structure of the atomic level. The Laplace transforms of the radial functions $\varphi_J^{(\pm)}(r, \omega)$ ($J=1/2, 3/2$), coincide, to within spin factors, with (10):

$$F_J^{(\pm)}(p, \omega) = \int_0^\infty dr e^{-pr} \varphi_J^{(\pm)}(r, \omega) = \eta_J^{E(\pm)} \Phi^{(\pm)}(p, \omega), \quad (21)$$

where

$$\begin{aligned} \eta_J^{E(+)} = & \frac{4}{\sqrt{3}} (-1)^{1+\mu} e^{-\mu} C_{1\mu 1/2m_J}^{Jm_J}, \\ \eta_J^{E(-)} = & \frac{4}{\sqrt{3}} (-1)^{1+\mu} e^{-\mu} C_{1\mu 1/2m_J}^{*Jm_J} \end{aligned}$$

($J=1/2, 3/2$), are the spin factors originating in the electric dipole interaction of the atom and the circularly polarized wave, with e_μ ($\mu=\pm 1, 0$) the cyclic components of the wave's polarization vector.

The correction $\Psi_{W,E}^{(2)}(\mathbf{r}, t)$ can also easily be found by analogy with (11) if we allow for the same radial dependence of the hyperfine operator in (4) (the noncentral part) and the spin-orbit coupling operator (16). The correction has the form

$$\begin{aligned} \Psi_{W,E}^{(2)}(\mathbf{r}, t) = & v_{(+)}(\mathbf{r}, \omega) \exp[-i(E^{(0)} + \omega)t] \\ & + v_{(-)}(\mathbf{r}, \omega) \exp[-i(E^{(0)} - \omega)t], \end{aligned} \quad (22)$$

$$v_{(\pm)}(\mathbf{r}, \omega) = \sum_{J=1/2}^{3/2} r^2 g_J^{(\pm)}(r, \omega) (Y_1(\mathbf{n}) \otimes \chi_{1/2})^{Jm_J}.$$

The Laplace transforms of the radial functions $g_J^{(\pm)}(r, \omega)$ are specified by the relationships:

$$\begin{aligned} P_J^{(\pm)}(p, \omega) = & \int_0^\infty dr e^{-pr} g_J^{(\pm)}(r, \omega) = \eta_J^{E(\pm)} \rho_J G^{(\pm)} \\ & \times (p, \omega) = \frac{\eta_J^{E(\pm)} \rho_J}{(p^2 - \kappa^2)^2} \left(\frac{p - \kappa}{p + \kappa} \right)^{1/\kappa} \int_\kappa^p dt (t^2 \\ & - \kappa^2) \left(\frac{t + \kappa}{t - \kappa} \right)^{1/\kappa} \int_t^\infty dt' \int_{t'}^\infty dt'' \Phi^{(\pm)}(t'', \omega), \end{aligned} \quad (23)$$

where $G^{(\pm)}(p, \omega)$ does not depend on spin variables,

$$\rho_J = (-1)^{J+1/2} \cdot 3 \begin{Bmatrix} 1 & 1 & 1 \\ 1/2 & 1/2 & J \end{Bmatrix}$$

is the spin factor, and $J=1/2, 3/2$.

Both the tensor polarizability (7) and the vector polarizability (19) are calculated by differentiating the Laplace transforms (21) and (23), following the scheme (13). In terms of Laplace variables we have

$$\alpha_v(\omega) = \alpha^2[\gamma(+\omega) - \gamma(-\omega)],$$

$$\gamma(\pm\omega) = -\frac{8}{3} \left\{ \Phi^{(\pm)}(p, \omega) + \frac{d}{dp} G^{(\pm)}(p, \omega) \right\} \Big|_{p=1}. \quad (24)$$

The functions $\Phi^{(\pm)}(p, \omega)$ have been defined in (10) and the derivatives $dG^{(\pm)}(p, \omega)/dp$ were found in deriving the tensor polarizability (14).

Formula (24) yields the following analytical expression for the vector polarizability of the ground $1S_{1/2}$ level of a hydrogenlike atom:

$$\alpha_v(\omega) = \alpha^2[\gamma(+\omega) - \gamma(-\omega)],$$

$$\gamma(\pm\omega) = \frac{2^9 \kappa^3}{(1+\kappa)^9} \left\{ {}_2F_1 \left(5, 2 - \frac{1}{\kappa}, 3 \right. \right.$$

$$\left. - \frac{1}{\kappa}, \left(\frac{1-\kappa}{1+\kappa} \right)^2 \right) \frac{1}{2-1/\kappa} - (1-\kappa) {}_2F_1 \left(5, 3 \right.$$

$$\left. - \frac{1}{\kappa}, 4 - \frac{1}{\kappa}, \left(\frac{1-\kappa}{1+\kappa} \right)^2 \right) \frac{1}{(3-1/\kappa)(1+\kappa)} \right\}$$

$$- \frac{2^8 \kappa^3}{9(1+\kappa)^{11}(2\kappa-1)(3\kappa-1)} \left\{ A(\kappa) \left[(3\kappa \right. \right.$$

$$\left. - 1)(6\kappa-1) \left(1 + \frac{1}{\kappa} \right)^2 - 2 {}_2F_1 \left(2, 3 - \frac{1}{\kappa}, 4 \right. \right.$$

$$\left. - \frac{1}{\kappa}, \frac{1-\kappa}{1+\kappa} \right) \right] + 2\kappa \sum_{\substack{n=2 \\ (n \neq 4)}}^6 B_n(\kappa) \left[(n \right.$$

$$\left. - 1) {}_2F_1 \left(n, 3 - \frac{1}{\kappa}, 4 - \frac{1}{\kappa}, \frac{1-\kappa}{1+\kappa} \right) \right.$$

$$\left. \times \frac{1}{(3\kappa-1)(1+\kappa)} - \frac{4}{1+\kappa} \left(\frac{1+\kappa}{2\kappa} \right)^n \right] \right\},$$

where the functions $A(\kappa)$ and $B_n(\kappa)$ ($n=2,3,5,6$) are defined in (15a).

4. CONCLUSION

As is well known (see, e.g., Refs. 10 and 23), the scalar dynamic polarizability of a hydrogenlike atom, $\alpha_s(\omega)$, can be written as a linear combination of the hypergeometric

functions ${}_2F_1$. The expressions for the dynamic tensor and vector polarizabilities, as Eqs. (15) and (25) show, contain both linear and quadratic combinations of ${}_2F_1$. The reason is that the corrections $\Psi_{hf,E}^{(2)}(\mathbf{r}, t)$ and $\Psi_{w,E}^{(2)}(\mathbf{r}, t)$, used in calculating $\alpha_t(\omega)$ and $\alpha_v(\omega)$, respectively, are solutions of inhomogeneous differential equations with the inhomogeneous term caused by the correction $\Psi_E^{(1)}(\mathbf{r}, t)$, which is responsible for $\alpha_s(\omega)$ (see Ref. 12).

In the static limit ($\omega \rightarrow 0$ and $\kappa \rightarrow 1$) the quantity $A(\kappa \rightarrow 1)$ is equal to $\frac{3}{2}$ the quantities $B_n(\kappa \rightarrow 1)$ ($n=2,3,5,6$) vanish,¹ and for the tensor polarizability (15) we obtain

$$\alpha_t(0) = \frac{47}{40} \sqrt{\frac{5}{F(F+1)(2F+3)(2F-1)}} (\alpha^2 \mu_N \eta_F^\mu + Q \eta_F^Q), \quad F=I \pm 1/2,$$

where the spin factors η_F^μ and η_F^Q are defined in (8a). For atomic hydrogen in the ground triplet state ($I=1/2, F=1$, and $Q=0$) this expression becomes the well-known result of Ref. 11:²

$$\alpha_t(0) = -\frac{47}{40} \alpha^2 \mu_N.$$

As for the vector polarizability (25), it is zero at $\omega=0$, in accordance with the properties (2). Its value for small finite frequencies can easily be obtained by expanding $\alpha_v(\omega)$ in a power series in ω . The two terms in the braces in (25) are caused by the relativistic correction to the dipole moment operator and by spin-orbit coupling. The expansion of the first of these terms yields a value of $-9\alpha^2\omega/2$ in an approximation linear in ω . A similar expansion of the second term yields $233\alpha^2\omega/72$. The net contribution of the two terms determines the vector polarizability of the $1S_{1/2}$ level of a hydrogenlike atom for low external-field frequencies:

$$\alpha_v(\omega \rightarrow 0) = -\frac{91}{72} \alpha^2 \omega,$$

which fully agrees with the results of Ref. 15. At the neodymium-laser frequency $\omega_N = 43.76 \times 10^{-3}$ at. units ($\lambda_N = 106 \times 10^{-6}$ cm) and the ruby-laser frequency $\omega_R = 66.79 \times 10^{-3}$ at. units ($\lambda_R = 69.43 \times 10^{-6}$ cm) this quantity is of order 10^{-6} at. units, following the numerical estimates made in Ref. 5.

Figure 1 depicts the functions $\alpha_t(\omega)$ and $\alpha_v(\omega)$ for the hydrogen ground state obtained numerically by tabulating the functions (15) (at $I=1/2, F=1$, and $Q=0$)³ and (25) and, for the sake of comparison, the scalar polarizability $\alpha_s(\omega)$ from Ref. 23. Note the various features of the frequency dependence of the tensor and vector polarizabilities. The presence of quadratic combinations of hypergeometric functions leads to a situation in which both $\alpha_t(\omega)$ and $\alpha_v(\omega)$ behave in the vicinity of poles (the resonance frequencies of the Lyman series) like even functions, in contrast to $\alpha_s(\omega)$, which in the vicinity of poles is an odd function. Moreover, at the frequency $\omega \sim 0.43$ at. units ($\lambda = 1.05 \times 10^{-5}$ cm), which lies within the range where the atomic-hydrogen medium is absolutely transparent

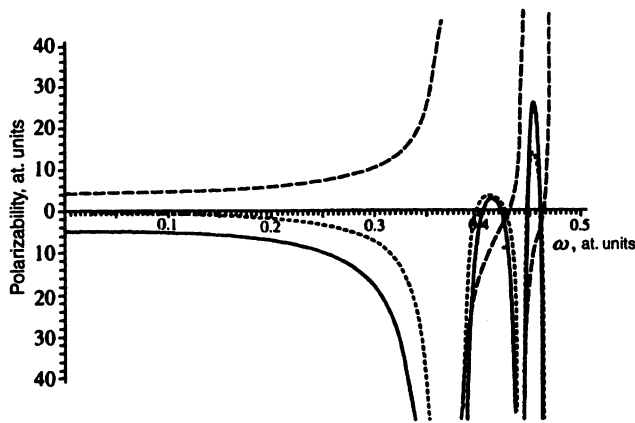


FIG. 1. The parameters $\alpha_s(\omega)$ (dashed curves), $\alpha_v(\omega)/\alpha^2$ (dotted curves), and $4\alpha_t(\omega)/\alpha^2\mu_N$ (solid curves) for the ground $1S_{1/2}$ level of atomic hydrogen.

($\alpha_s(\omega)=0$) if we ignore the tensor polarizability, the quantity $\alpha_t(\omega)$ is finite and exceeds the static value by a factor of almost three.

1) Actually, the divergence of $B_5(\kappa)$ and $B_6(\kappa)$ as $\kappa \rightarrow 1$ is fictitious and can be removed by l'Hôpital's rule.

2) Note, however, that Sandars¹¹ used a somewhat different definition of the spin part of the polarizability operator (1). Hence $\alpha_{12}=2\alpha_t/3$, where (α_{12} is the tensor polarizability in Sandars's notation¹¹).

3) We obtained this diagram earlier in Ref. 12.

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