Relativistic dynamical polarizability of hydrogen-like atoms

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Abstract. Using the operator representation of the Dirac Coulomb Green function the analytical method in perturbation theory is employed in obtaining solutions of the Dirac equation for a hydrogen-like atom in a time-dependent electric field. The relativistic dynamical polarizability of hydrogen-like atoms is calculated and analysed.

1. Introduction

In stationary perturbation theory as well as in the time-dependent one, the method of using the Coulomb Green function has found wide application in obtaining analytical solutions of the Schrödinger or Dirac equations. The main advantage of this method is the possibility of obtaining the final results in closed analytical form or reducing results to the summation of rapidly convergent series. Therefore, by using the above-mentioned method one can avoid a lot of complex numerical integrations (see, for example, Makhanek and Korol'kov 1982, Zapryagaev et al 1985 and references cited therein). On the basis of the application of the connection between the problem of the four-dimensional isotropic harmonic oscillator and that of a hydrogen-like atom in electromagnetic fields (see Kustaanheimo and Stiefel 1965), it has been proposed to establish a new representation of the Coulomb Green function in the form of a product of annihilation and creation operators (this is called by us an operator representation). Operator representation of the Coulomb Green functions is very efficient in applications for the non-relativistic case (Le Van Hoang *et al* 1989) as well as for the relativistic one (Le Anh Thu et al 1994). The main elements of the algebraic method used (with the aid of the operator representation of the Coulomb Green functions) in Le Van Hoang et al (1989) and in Le Anh Thu et al (1994) are as follows. By using the above-mentioned connection, all operators of the algebra of the dynamical symmetry group SO(4, 2) can be found in the quadratic form of the annihilation and creation operators (see, for example, Kleinert 1968, Komarov and Romanova 1982). Therefore, the calculation method, based on the use of the algebra of SO(4, 2), leads only to the use of the simple commutation relations between the latter operators. The use of this method together with the operator representation of the Coulomb Green function, therefore essentially reduces the calculation process and provides for reducing rather complicated calculations of matrix elements with Coulomb wavefunctions to a purely algebraic procedure of transforming the product of the annihilation and creation operators to the normal form. The advantages of the

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proposed algebraic method are found not only in the simplicity of the calculation process but also in the possibility of obtaining the final results in the summation of rapidly convergent series. In fact, some clever results are obtained in Le Anh Thu et al (1994) for the problem of calculation of the relativistic polarizability of hydrogen-like atoms. In this present paper, we consider the problem of calculating the relativistic polarizability of the ground state of hydrogen-like atoms on the basis of application of the operator representation of the Dirac Coulomb Green function established in Le Anh Thu et al (1994). These calculations, besides their purely theoretical significance, are of great practical interest connected with recent developments in experimental investigations of multiply charged ions (see, for example, Zapryagaev et al 1985, Paratzacos and Mork 1979). However, the majority of accurate calculations has been done only for the static polarizability of relativistic hydrogen-like atoms (see also Drake and Goldman 1981, 1988, Johnson et al 1988). In our calculations the radiation corrections are neglected, taking into account the fact that this effect is small compared with the external field effects. Our results are directly generalized from the nonrelativistic calculations (Zapryagaev et al 1985) and coincide with the results in the static limit (Le Anh Thu et al 1994).

2. Equation in two-dimensional complex space

The Dirac equation for a hydrogen-like atom in the field of linearly polarized light can be written as follows ($\hbar = m = c = 1$):

$$\left(-\mathrm{i}\alpha_{\lambda}r\frac{\partial}{\partial x_{\lambda}}+\beta r-Ze^{2}+\frac{\theta}{2}erx_{3}(\mathrm{e}^{\mathrm{i}\nu t}+\mathrm{e}^{-\mathrm{i}\nu t})\right)\Psi(\boldsymbol{r},t)=\mathrm{i}r\frac{\partial\Psi(\boldsymbol{r},t)}{\partial t}\qquad(1)$$

where α_{λ} ($\lambda = 1, 2, 3$) and β are the Dirac matrices; θ and ν are the amplitude and frequency of the external electric field respectively. Further on, we use the usual representation

$$\Psi = \begin{pmatrix} \Psi_1 \\ \Psi_2 \end{pmatrix}$$
 $lpha_{\lambda} = \begin{pmatrix} 0 & \sigma_{\lambda} \\ \sigma_{\lambda} & 0 \end{pmatrix}$ $eta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

where Ψ_1 and Ψ_2 are two-component spinors and σ_{λ} ($\lambda = 1, 2, 3$) are the Pauli matrices. The formal changes (see Le Anh Thu *et al* 1994)

$$x_{\lambda} \to (\sigma_{\lambda})_{st} \xi_s^* \xi_t \qquad r \to \xi_s^* \xi_s \qquad r \hat{p}_{\lambda} \to -\frac{i}{2} (\sigma_{\lambda})_{st} \left(\xi_t \frac{\partial}{\partial \xi_s} + \xi_s^* \frac{\partial}{\partial \xi_t^*} \right)$$
(2)

reduce equation (1) to an equation describing the interaction between a 'particle' with complex coordinates ξ_s (s = 1, 2) and the external variable electric field. Here, in (2) summation is indicated by means of repeated indices. The scalar product of wavefunctions in ξ -space is defined by the correlation

$$\langle \tilde{\Psi} \mid \tilde{\varphi} \rangle = \int_{-\infty}^{+\infty} \mathrm{d}\xi_1' \int_{-\infty}^{+\infty} \mathrm{d}\xi_1'' \int_{-\infty}^{+\infty} \mathrm{d}\xi_2' \int_{-\infty}^{+\infty} \mathrm{d}\xi_2'' \tilde{\Psi}^*(\xi_1', \xi_1'', \xi_2', \xi_2'') \tilde{\varphi}(\xi_1', \xi_1'', \xi_2', \xi_2'')$$
(3)

where $\xi'_s \equiv \text{Re}\xi_s$, $\xi''_s \equiv \text{Im}\xi_s$. All operators appearing in (1) are henceforth considered to conform with the formal changes (2). Thus, the operator on the left-hand side of equation (1) is self-adjoint with respect to the scalar product of wavefunctions defined by (3).

We will solve equation (1) by using the method of perturbation theory assuming the external electric field to be small. Its solution can be found in the form

$$\Psi(\mathbf{r},t) = \Psi^{(0)}(\mathbf{r},t) + \theta \Psi^{(-)}(\mathbf{r},t)$$

= $\Psi^{(0)}(\mathbf{r}) e^{-i\varepsilon_0 t} + \theta u(\mathbf{r}) e^{-it(\varepsilon_0 - \nu)} + \theta v(\mathbf{r}) e^{-it(\varepsilon_0 + \nu)}$ (4)

where $\Psi^{(0)}(\mathbf{r})$ is a wavefunction in the zero-order approximation, i.e. a solution of the Dirac equation

$$\left(-\mathrm{i}\alpha_{\lambda}r\frac{\partial}{\partial x_{\lambda}}+\beta r-\varepsilon_{0}r\right)\Psi^{(0)}(r)=Ze^{2}\Psi^{(0)}(r)$$
(5)

and ε_0 is the energy in the zero-order approximation. By substituting (4) into (1) and taking into account (5), we obtain the equations

$$\left(-\mathrm{i}\alpha_{\lambda}r\frac{\partial}{\partial x_{\lambda}}+\beta r-Ze^{2}\right)u(r)-r(\varepsilon_{0}-\nu)u(r)=-\frac{1}{2}erx_{3}\Psi^{(0)}(r) \tag{6}$$

$$\left(-\mathrm{i}\alpha_{\lambda}r\frac{\partial}{\partial x_{\lambda}}+\beta r-Ze^{2}\right)v(r)-r(\varepsilon_{0}+\nu)v(r)=-\frac{1}{2}erx_{3}\Psi^{(0)}(r).$$
(7)

Noting that equations (6) and (7) have the same structure, we consider only equation (6) for the function u(r); then by replacing -v by v in u(r) we find the function v(r).

Let us now present $u(\mathbf{r})$ and $\Psi^{(0)}$ in the form

$$u = \begin{pmatrix} \varphi_1^{(1)} \\ (\sigma_\lambda x_\lambda/r)\varphi_2^{(1)} \end{pmatrix} \qquad \Psi^{(0)} = \begin{pmatrix} \varphi_1^{(0)} \\ (\sigma_\lambda x_\lambda/r)\varphi_2^{(0)} \end{pmatrix}.$$
(8)

The substitution of (8) into (6) leads to the following set of equations for $\varphi_1^{(1)}$ and $\varphi_2^{(1)}$:

$$-i\left(x_{\lambda}\frac{\partial}{\partial x_{\lambda}}+1\right)\varphi_{2}^{(1)}-i\hat{\kappa}\varphi_{2}^{(1)}+r(1-\varepsilon_{0}+\nu)\varphi_{1}^{(1)}-Ze^{2}\varphi_{1}^{(1)}=-\frac{1}{2}erx_{3}\varphi_{1}^{(0)}$$
(9)

$$-i\left(x_{\lambda}\frac{\partial}{\partial x_{\lambda}}+1\right)\varphi_{1}^{(1)}+i\hat{\kappa}\varphi_{1}^{(1)}-r(1+\varepsilon_{0}-\nu)\varphi_{2}^{(1)}-Ze^{2}\varphi_{2}^{(1)}=-\frac{1}{2}erx_{3}\varphi_{2}^{(0)}$$
(10)

where $\hat{\kappa} = 1 + \sigma_{\lambda} \hat{l}_{\lambda}$; \hat{l} is the orbital momentum operator.

By using the transformations

$$\varphi_1^{(0)} = -\frac{1}{2}i\sqrt{1+\varepsilon_0}(\mathcal{F}^{(0)} - \mathcal{G}^{(0)}) \qquad \varphi_2^{(0)} = \frac{1}{2}\sqrt{1-\varepsilon_0}(\mathcal{F}^{(0)} + \mathcal{G}^{(0)}) \quad (11.1)$$

and

$$\varphi_1^{(1)} = -\frac{1}{2}i\sqrt{1+\varepsilon_0 - \nu}(\mathcal{F}^{(1)} - \mathcal{G}^{(1)}) \qquad \varphi_2^{(1)} = \frac{1}{2}\sqrt{1-\varepsilon_0 + \nu}(\mathcal{F}^{(1)} + \mathcal{G}^{(1)})$$
(11.2)

we find

$$\left[x_{\lambda}\frac{\partial}{\partial x_{\lambda}} + 1 + \omega r - \frac{Ze^{2}}{\omega}(\varepsilon_{0} - \nu)\right]\mathcal{F}^{(1)} + \left(\hat{\kappa} + \frac{Ze^{2}}{\omega}\right)\mathcal{G}^{(1)} = rx_{3}(\tilde{A}_{-}\mathcal{F}^{(0)} + \tilde{A}_{+}\mathcal{G}^{(0)}) \quad (12)$$

$$\left[x_{\lambda}\frac{\partial}{\partial x_{\lambda}}+1-\omega r+\frac{Ze^{2}}{\omega}(\varepsilon_{0}-\nu)\right]\mathcal{G}^{(1)}+\left(\hat{\kappa}-\frac{Ze^{2}}{\omega}\right)\mathcal{F}^{(1)}=-rx_{3}(\tilde{A}_{+}\mathcal{F}^{(0)}+\tilde{A}_{-}\mathcal{G}^{(0)})$$
(13)

where

$$\omega = \sqrt{1 - (\varepsilon_0 - \nu)^2}$$
$$\tilde{A}_{\pm} = \frac{e}{4\omega} [\sqrt{(1 - \varepsilon_0)(1 - \varepsilon_0 + \nu)} \pm \sqrt{(1 + \varepsilon_0)(1 + \varepsilon_0 - \nu)}].$$
(14)

After expanding the functions \mathcal{F} and \mathcal{G} in power series of the eigenfunctions of operators \hat{L}^2 and $\hat{\kappa}$, the operator $\hat{\kappa}$ appearing in (12) and (13) becomes a *c*-number and, therefore, in order to solve equations (12) and (13) we can employ the Green function method established in Le Anh Thu *et al* (1994). In the next section we will show an example by calculating the dynamical polarizability of hydrogen-like atoms in the ground state.

3. Relativistic dynamical polarizability in the ground state of hydrogen-like atoms

The solution of equation (5) can be easily obtained by purely algebraic calculations. In particular, we can find for the ground state the solution (see Komarov and Romanova 1985):

$$\mathcal{F}^{(0)} = \frac{(2\omega_0)^{\varepsilon_0 - 1}}{\sqrt{\Gamma(2\varepsilon_0)}} r^{\varepsilon_0 - 1} |0(\omega_0)\rangle \chi^{\uparrow} \qquad \mathcal{G}^{(0)} = 0$$
(15)

where $\omega_0 = Ze^2$; $\varepsilon_0 = \sqrt{1 - (Ze^2)^2}$; $\chi^{\uparrow(\downarrow)}$ are eigenvectors of operator σ_3 and $|0(\omega_0)\rangle$ is the vacuum state defined by the equations

$$a_s(\omega_0)|0(\omega_0)\rangle = b_s(\omega_0)|0(\omega_0)\rangle = 0 \qquad s = 1, 2.$$

Here the operators $a_s(\omega)$, $b_s(\omega)$ are defined as follows

$$a_{s}(\omega) = \sqrt{\frac{\omega}{2}} \left(\xi_{s} + \frac{1}{\omega} \frac{\partial}{\partial \xi_{s}^{*}} \right) \qquad b_{s}(\omega) = \sqrt{\frac{\omega}{2}} \left(\xi_{s}^{*} + \frac{1}{\omega} \frac{\partial}{\partial \xi_{s}} \right)$$
$$a_{s}^{+}(\omega) = \sqrt{\frac{\omega}{2}} \left(\xi_{s}^{*} - \frac{1}{\omega} \frac{\partial}{\partial \xi_{s}} \right) \qquad b_{s}^{+}(\omega) = \sqrt{\frac{\omega}{2}} \left(\xi_{s} - \frac{1}{\omega} \frac{\partial}{\partial \xi_{s}^{*}} \right)$$

where ω is a positive parameter (see Le Anh Thu *et al* 1994). The perturbation term in equations (12) and (13) thus has the form

$$\pm \tilde{A}_{\mp} r x_3 \mathcal{F}^{(0)} = \pm A_{\mp} r^{\varepsilon_0} (Z_{1,-1} + \sqrt{2} Z_{1,2}) |0(\omega_0)\rangle.$$
(16)

Here, we use the notation

$$A_{\pm} = \frac{\sqrt{6}(2\omega_0)^{\varepsilon_0 - 2}}{\sqrt{\Gamma(2\varepsilon_0)}}\tilde{A}_{\pm}$$

and $Z_{l,\kappa}$ are eigenvectors of (i) the square orbital momentum operator and (ii) the operator $\hat{\kappa}$. The structure of the perturbation term (16) prompts us to find the solution in the form

$$\mathcal{F}^{(1)} = \sum_{\kappa = -1,2} \mathcal{F}^{(1)}_{\kappa} \qquad \mathcal{G}^{(1)} = \sum_{\kappa = -1,2} \mathcal{G}^{(1)}_{\kappa}$$
(17)

where $\mathcal{F}_{\kappa}^{(1)}$ and $\mathcal{G}_{\kappa}^{(1)}$ satisfy the equations

$$\begin{bmatrix} x_{\lambda} \frac{\partial}{\partial x_{\lambda}} + 1 + \omega r - \frac{Ze^{2}}{\omega} (\varepsilon_{0} - \nu) \end{bmatrix} \mathcal{F}_{\kappa}^{(1)} + \left(\kappa + \frac{Ze^{2}}{\omega}\right) \mathcal{G}_{\kappa}^{(1)} = A_{-} \sqrt{|\kappa|} r^{\varepsilon_{0}} Z_{1\kappa} |0(\omega_{0})\rangle, \quad (18)$$
$$\begin{bmatrix} x_{\lambda} \frac{\partial}{\partial x_{\lambda}} + 1 - \omega r + \frac{Ze^{2}}{\omega} (\varepsilon_{0} - \nu) \end{bmatrix} \mathcal{G}_{\kappa}^{(1)} + \left(\kappa - \frac{Ze^{2}}{\omega}\right) \mathcal{F}_{\kappa}^{(1)} = -A_{+} \sqrt{|\kappa|} r^{\varepsilon_{0}} Z_{1\kappa} |0(\omega_{0})\rangle. \quad (19)$$

From (19) it follows that

$$\mathcal{F}_{\kappa}^{(1)} = -\frac{A_{+}\sqrt{|\kappa|}}{\kappa - Ze^{2}/\omega}r^{\varepsilon}Z_{1\kappa}|0(\omega_{0})\rangle - \frac{1}{\kappa - Ze^{2}/\omega}\left[x_{\lambda}\frac{\partial}{\partial x_{\lambda}} + 1 - \omega r + \frac{Ze^{2}}{\omega}(\varepsilon_{0} - \nu)\right]\mathcal{G}_{\kappa}^{(1)}.$$
(20)

By substituting (20) into (18) we obtain:

$$\left\{-\left[x_{\lambda}\frac{\partial}{\partial x_{\lambda}}+1+\omega r-\frac{Ze^{2}}{\omega}(\varepsilon_{0}-\nu)\right]\left[x_{\lambda}\frac{\partial}{\partial x_{\lambda}}+1-\omega r+\frac{Ze^{2}}{\omega}(\varepsilon_{0}-\nu)\right]\right.\\\left.+\kappa^{2}-\left(\frac{Ze^{2}}{\omega}\right)^{2}\right\}\mathcal{G}_{\kappa}^{(1)}$$

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$$= A_{-}\sqrt{|\kappa|} \left(\kappa - \frac{Ze^{2}}{\omega}\right) r^{\varepsilon_{0}} Z_{1\kappa}|0(\omega_{0})\rangle + A_{+}\sqrt{|\kappa|} \\ \times \left[x_{\lambda}\frac{\partial}{\partial x_{\lambda}} + 1 + \omega r - \frac{Ze^{2}}{\omega}(\varepsilon_{0} - \nu)\right] r^{\varepsilon_{0}} Z_{1\kappa}|0(\omega_{0})\rangle.$$
(21)

As mentioned above (see (2)), all operators in (20), (21) (though formally written for brevity via the usual coordinates x_{λ} ($\lambda = 1, 2, 3$)) are understood in the sense of the formal changes (2). These changes are equivalent to the transformation from *r*-space to ξ -space (Kustaanheimo-Stiefel transformation, see Kustaanheimo and Stiefel (1965)):

$$\begin{cases} x_{\lambda} = \xi_s^*(\sigma_{\lambda})_{st}\xi_t & (s, t = 1, 2) \\ \chi = \arg(\xi_1) \end{cases}$$

So we can rewrite the operators used in (20), (21) via the annihilation and creation operators as follows:

$$x_{\lambda}\frac{\partial}{\partial x_{\lambda}} = \frac{M(\omega)}{2} - \frac{M^{+}(\omega)}{2} - 1 \qquad r = \frac{1}{2\omega}[M(\omega) + M^{+}(\omega) + N(\omega) + 2]$$

where the notations

$$N = a_s^+ a_s + b_s^+ b_s \qquad M = a_s b_s \qquad M^+ = a_s^+ b_s^+.$$

Therefore, equation (21) has a more convenient form

$$\begin{cases} \left[M + \frac{1}{2}N + 1 - \frac{Ze^2}{\omega}(\varepsilon_0 - \nu) \right] \left[M^+ + \frac{1}{2}N + 1 - \frac{Ze^2}{\omega}(\varepsilon_0 - \nu) \right] + \kappa^2 - \left(\frac{Ze^2}{\omega}\right)^2 \right\} |\mathcal{G}_{\kappa}^{(1)}\rangle \\ = A_- \sqrt{|\kappa|} \left(\kappa - \frac{Ze^2}{\omega} \right) r^{\varepsilon_0} Z_{1\kappa} |0(\omega_0)\rangle \\ + A_+ \sqrt{|\kappa|} \left[M + \frac{1}{2}N + 1 - \frac{Ze^2}{\omega}(\varepsilon_0 - \nu) \right] r^{\varepsilon_0} Z_{1\kappa} |0(\omega_0)\rangle. \tag{22}$$

Here and henceforth, we omit for brevity the parameter ω in the expressions of the operators. Equation (22) has the same structure as the equations appearing in the case of calculation of the static polarizability of hydrogen-like atoms (see Le Anh Thu *et al* 1994). The only difference is in the perturbation term on the left-hand side of these equations. Therefore, we can by analogy find the solutions of equation (22), using the Green function operator which, according to Le Anh Thu *et al* (1994), can be established as follows:

$$\hat{G}_{l\kappa} = \hat{B}_{l\kappa} \frac{1}{2 + N + M + M^+} \qquad \hat{B}_{l\kappa} = \sum_{s=0}^{\infty} d_s (N/2) M^s$$
(23)

where

$$d_{0}(n) = -\frac{1}{n + \gamma + 2 - Ze^{2}\varepsilon/2}$$

$$d_{s}(n) = (-1)^{s}(2\gamma + 1)\frac{(n + l + 1)!}{(n + s + l + 1)!} \frac{\Gamma(n + s + 1 - \gamma - Ze^{2}\varepsilon/2)}{\Gamma(n + 2 - \gamma - Ze^{2}\varepsilon/\omega)}$$

$$\times \frac{\Gamma(n + 2 + \gamma - Ze^{2}\varepsilon/2)}{\Gamma(n + s + 3 + \gamma - Ze^{2}\varepsilon/2)} \qquad s = 1, 2, 3...$$

$$\gamma = -l - 1 + \sqrt{\kappa^{2} - Z^{2}e^{4}} \qquad \varepsilon = \varepsilon_{0} - \nu.$$
(24)

Here, we note that the Green function operator (23) acts on the basis of states with frequency ω . However, the wavefunctions in the zero-order approximation (15) have the frequency

 $\omega_0 = Ze^2$. Therefore, in order to use the algebraic calculation we have to transform the wavefunctions (15) from the frequency ω_0 to ω using the unitary transformation (see Komarov and Romanova 1982):

$$|\Phi(\omega_0)\rangle = \hat{U}(\omega_0, \omega)|\Phi(\omega)\rangle,$$

where

$$\hat{U}(\omega_0,\omega) = \exp\left\{\frac{1}{2}\ln\frac{\omega_0}{\omega}[M(\omega) - M^+(\omega)]\right\}.$$

This transformation can be reduced to the normal form

$$\hat{U}(\omega_0, \omega) = \frac{4\omega_0\omega}{(\omega_0 + \omega)^2} \exp\left(\frac{\omega - \omega_0}{\omega + \omega_0} M^+(\omega)\right) \exp\left(N(\omega) \ln \frac{2\sqrt{\omega\omega_0}}{\omega + \omega_0}\right) \\ \times \exp\left(-\frac{\omega - \omega_0}{\omega + \omega_0} M(\omega)\right).$$
(25)

Finally, by analogy with what was done in Le Anh Thu *et al* (1994) for the same equation, we find the solution

$$\begin{aligned} |\mathcal{G}_{\kappa}^{(1)}\rangle &= A_{-}\sqrt{|\kappa|} \left(\kappa - \frac{Ze^{2}}{\omega}\right) r^{\gamma} \hat{G}_{1\kappa} r^{\varepsilon_{0}-\gamma} \hat{U}(\omega_{0},\omega) Z_{1\kappa} |0(\omega_{0})\rangle + A_{+}\sqrt{|\kappa|} r^{\gamma} \hat{G}_{1\kappa} r^{-\gamma} \\ &\times \left[M + \frac{N}{2} + 1 - \frac{Ze^{2}}{\omega} (\varepsilon_{0}-\nu)\right] r^{\varepsilon_{0}} \hat{U}(\omega_{0},\omega) Z_{1\kappa} |0(\omega_{0})\rangle. \end{aligned}$$
(26)

The wavefunction $|\mathcal{F}_{\kappa}^{(1)}\rangle$ can be obtained by substituting (26) into (20).

Let us now calculate the dynamical polarizability of the ground state of hydrogen-like atoms, the formula of which in ξ -space has the form

$$a(\nu) = 2 \frac{\langle \Psi^{(0)} | erx_3 | \Psi^{(1)} \rangle}{\langle \Psi^{(0)} | r | \Psi^{(0)} \rangle}.$$

This formula, after considering (8), (11), (15) and (17), can be written as follows

$$a(v) = \sum_{\kappa = -1, 2} a_{\kappa}(v)$$

where

$$a_{\kappa}(\nu) = \frac{4\omega_0 \omega \sqrt{|\kappa|}}{\varepsilon_0} \langle 0(\omega_0) | Z_{1\kappa} r^{\varepsilon_0} | A_+ \mathcal{F}_{\kappa}^{(1)} + A_- \mathcal{G}_{\kappa}^{(1)} \rangle.$$
(27)

By substituting the found solutions (20), (26) into (27) we find the expression for the positive frequency term of polarizability

$$a_{\kappa}(+\nu) = \frac{4\omega_{0}\omega|\kappa|}{\varepsilon_{0}} \left\{ \frac{A_{+}^{2}}{B} \langle 0|r^{2\varepsilon_{0}}|0\rangle + \left[A_{-}^{2}B + 2A_{+}A_{-}\delta + \frac{A_{+}^{2}\delta^{2}}{B}\right] H_{00}^{\kappa} + \frac{4\omega(\omega-\omega_{0})}{(\omega+\omega_{0})^{2}} \left[A_{+}A_{-} + \frac{A_{+}^{2}\delta}{B}\right] H_{01}^{\kappa} + \frac{4\omega^{2}(\omega-\omega_{0})^{2}}{(\omega+\omega_{0})^{4}} \frac{A_{+}^{2}}{B} H_{11}^{\kappa} \right\}.$$
 (28)

Here, we use the notations

$$B = \kappa - \frac{Ze^2}{\omega} \qquad \delta = \frac{4(\omega - \omega_0)}{\omega + \omega_0} - \frac{Ze^2}{\omega} (\varepsilon_0 - \nu) + \varepsilon_0 + 2$$

$$H_{nm}^{\kappa} = \langle 0(\omega) | Z_{1\kappa} \hat{U}^+(\omega_0, \omega) M^n r^{\varepsilon_0 + \gamma} \hat{G}_{\kappa} r^{\varepsilon_0 - \gamma} (M^+)^m \hat{U}(\omega_0, \omega) Z_{1\kappa} | 0(\omega) \rangle.$$
(29)

A similar expression for the negative frequency term can be obtained by replacing v by -v in formulae (14), (18), (19).



Figure 1. (a) The dependence of the dynamical polarizability of the hydrogen-like atom (Z = 50) on the frequency v of the external field (one line (A) is shown in figure 1(b) with large scale). (b) The line (A) of figure 1(a) on a larger scale.

By using the algebra of operators M^+ , M, N:

 $[M, M^+] = N + 2$ [M, N + 2] = 2M $[N + 2, M^+] = 2M^+$

and the correlations

$$N(M^{+})^{n} Z_{l\kappa} |0\rangle = 2(n+l)(M^{+})^{n} Z_{l\kappa} |0\rangle$$

$$M(M^{+})^{n} Z_{l\kappa} |0\rangle = n(n+2l+1)(M^{+})^{n-1} Z_{l\kappa} |0\rangle$$



Figure 2. The dependence of the dynamical polarizability of the hydrogen-like atom (Z = 100) on the frequency ν of the external field.

$$r^{\rho} Z_{l\kappa} |0\rangle = \frac{\Gamma(\rho + 2l + 2)}{(2\omega)^{\rho} \Gamma(-\rho)} \sum_{s=0}^{\infty} \frac{(-1)^{s}}{s!} \frac{\Gamma(s-\rho)}{(s+2l+1)!} (M^{+})^{s} Z_{l\kappa} |0\rangle$$

we algebraically obtained the explicit form of the term H_{nm}^{κ} as follows:

$$H_{nm}^{\kappa} = \frac{1}{12\omega} \left(\frac{2\sqrt{\omega_0 \omega}}{\omega_0 + \omega} \right)^8 (\omega_0 + \omega)^{1-2\varepsilon_0} \sum_{p=0}^{\infty} (p+3)!$$

$$\times \sum_{q=0}^p (-1)^q \binom{p}{q} \frac{\Gamma(q+\varepsilon_0 - \gamma)\Gamma(q+3+\varepsilon_0 - \gamma)}{\Gamma(q+\varepsilon_0 - \gamma - m)(q+3)!}$$

$$\times \sum_{s=0}^p (-1)^s \frac{d_s(p-s+1)}{(p-s)!}$$

$$\times \sum_{t=0}^{p-s} (-1)^t \binom{p-s}{t} \left(\frac{2\omega}{\omega+\omega_0} \right)^{t+q-n-m}$$

$$\times \frac{\Gamma(t+1+\varepsilon_0+\gamma)\Gamma(t+4+\varepsilon_0+\gamma)}{\Gamma(t+1+\varepsilon_0+\gamma-n)(t+3)!}.$$
(30)

Direct calculations show that all power series appearing in the term H_{nm}^{κ} are rapidly convergent. The high convergency of these power series is directly related to the expansion (23) of the Dirac Coulomb Green function which, in fact, is established on the basis of harmonic oscillator wavefunctions. Moreover, the expression (28) for the polarizability contains only H_{nm}^{κ} with n, m = 0, 1, the calculation of which needs only some of the first terms in the summation over p. For example, for frequency v less than the fourth resonance frequency (relative to the transition from the ground state to the $3P_{3/2}$ state) the contribution of the terms with p = 0, 1 in H_{nm}^{κ} (n, m = 0, 1) is about 98–99% for all $Z \leq 137$.

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In figures 1(a) and (b) the dependence of relativistic polarizability on the external field frequency is given for hydrogen-like atoms with Z = 50. The dotted lines correspond to the non relativistic limit case. Figure 2 gives the same for Z = 100.

Let us now consider the non-relativistic limit, i.e. take into account only the first term in the expansion in the power series of Ze^2 . For this case, we can effect summation over the variables t, q, s in the expression of H_{nm}^{κ} and then have H_{nm}^{κ} in the form of hypergeometric functions. Consequently, we have

$$a_{\text{non}}(\pm\nu) = \frac{2^{11}\mu^3 e^2}{(Ze^2)^4(\mu+1)^{10}} \left\{ \frac{1}{(2-1/\mu)(3-1/\mu)} \, {}_2F_1\left(5,2-\frac{1}{\mu},4-\frac{1}{\mu},\left(\frac{\mu-1}{\mu+1}\right)^2\right) + \frac{5\mu^2}{(\mu+1)^2(3-1/\mu)} \, {}_2F_1\left(6,3-\frac{1}{\mu},4-\frac{1}{\mu},\left(\frac{\mu-1}{\mu+1}\right)^2\right) \right\}$$
(31)

where $\mu = \sqrt{1 \pm 2\nu/(Ze^2)^2}$. This expression coincides with the well known result obtained by Vetchinkin and Khristenko (1968).

By putting $\nu = 0$ into (28), (30) and (31) we thus find the formula for the relativistic polarizability. It is easy to see that for $\omega = \omega_0$ the formula (28) contains only the term H_{00}^{κ} . Taking into account the formula (Prudnikov *et al* 1981)

$$\sum_{k=0}^{n} (-1)^k \binom{n}{k} \binom{a+k}{m} = (-1)^n \binom{a}{m-n}$$

we can lead H_{00}^{κ} to the form

$$H_{00}^{\kappa} = \frac{1}{6(2\omega_0)^{2\varepsilon_0}} \Gamma(\varepsilon_0 - \gamma) \Gamma(\varepsilon_0 - \gamma + 3) \Gamma(\varepsilon_0 + \gamma + 1) \Gamma(\varepsilon_0 + \gamma + 4) \sum_{p=0}^{\infty} \frac{1}{\Gamma(\varepsilon_0 - \gamma - p)} \times \sum_{s=0}^{p} \frac{d_s(p-s+1)}{(p-s)!(p-s+3)!\Gamma(\varepsilon_0 + \gamma + 1 - p + s)}.$$
(32)

The substitution of (32) into (28) gives for v = 0 the relativistic static polarizability

$$a = \frac{e^{2}(\varepsilon_{0}+1)(2\varepsilon_{0}+1)(4\varepsilon_{0}^{2}+13\varepsilon_{0}+12)}{36\omega_{0}^{4}} - \frac{e^{2}(\varepsilon_{0}-2)^{2}\Gamma(\varepsilon_{0}+\gamma+4)\Gamma(\varepsilon_{0}-\gamma+3)}{36\omega_{0}^{4}\Gamma(2\varepsilon_{0})\Gamma(-\varepsilon_{0}-\gamma)\Gamma(1-\varepsilon_{0}+\gamma)} \times \left[\sum_{k=0}^{\infty} \frac{\Gamma(k-\varepsilon_{0}-\gamma)\Gamma(k-\varepsilon_{0}+\gamma+1)}{k!(k+3)!(k-\varepsilon_{0}+\gamma+3)} - (2\gamma+1) + \sum_{q=1}^{\infty} \frac{\Gamma(q-\varepsilon_{0}+\gamma+1)}{(q+3)!} \frac{\Gamma(q-\varepsilon_{0}-\gamma+2)}{\Gamma(q-\varepsilon_{0}+\gamma+4)} + \sum_{s=0}^{\infty} \frac{\Gamma(s-\varepsilon_{0}-\gamma)\Gamma(s-\varepsilon_{0}+\gamma+3)}{s!\Gamma(s-\varepsilon_{0}-\gamma+3)}\right]$$

where $\gamma = -2 + \sqrt{4 - (Ze^2)^2}$. This result absolutely coincides with the result obtained in Le Anh Thu *et al* (1994) (see also Barut and Nagel 1976).

4. Conclusion

In conclusion we would like to note that the magnetic field effects, as a rule, should be taken into account for a detailed investigation of the behaviour of a relativistic atom in the field of linearly polarized light. These effects can be neglected only in the non-relativistic limit. 2906 Le Anh Thu et al

The above method proposed with the use of the operator representation of the Coulomb Green function can also be employed, for example, in calculating magnetic polarizability. Consideration of magnetic field effects leads only to an enormous number of calculations, which are more complicated in comparison with the above calculations but could be done analogously by analytical methods. Moreover, we hope that our algebraic method would be helpful when considering the problem of an atom in a quantum field, in particular in calculating the Lamb shift of multiply charged ions, which is of great interest and has been widely investigated recently (see, for example, Snyderman 1991).

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References

- Barut A O and Nagel J 1976 Phys. Rev. D 13 2075
- Drake G W F and Goldman S P 1981 Phys. Rev. A 23 2093
- Johnson W R, Blundell S A and Sapirstein J 1988 Phys. Rev. A 37 307
- Kleinert H 1968 Lectures in Theoretical Physics ed W E Brittin and A O Barut (New York: Gordon and Breach) p 427
- Komarov L I and Romanova T S 1982 Izv. Acad. Nauk BSSR, Ser. Fiz. Mat. Nauk 2 98
- Kustaanheimo P and Stiefel E 1965 J. Reine Angrew. Math. 218 204
- Le Anh Thu, Le Van Hoang, Komarov L I and Romanova T S 1994 J. Phys. B: At. Mol. Opt. Phys. 27 4083
- Le Van Hoang, Komarov L I and Romanova T S 1989 J. Phys. A: Math. Gen. 22 1543
- Makhanek A G and Korol'kov V C 1982 Analytical Methods in the Quantum Perturbation Theory (Minsk: Nauka i Tekcnika)
- Paratzacos P and Mork K 1979 Phys. Rep. C 21 81
- Prudnikov A P, Brichkov Yu A and Marichev O I 1981 Integrals and Series (Moscow: Nauka)
- Snyderman N J 1991 J. Ann. Phys. 211 43
- Vetchinkin S I and Khristenko S V 1968 Opt. Spectrosc. 25 650
- Zapryagaev S A, Manakov N L and Pal'chikov V G 1985 Ehtoery of Multiply Charged Ions with One or Two Electrons (Moscow: Energoatomizdat)
- Zon B A, Manakov N L and Rapoport L P 1972 Yad. Phys. 15 508