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Operator representation of the Dirac Coulomb Green function and relativistic polarizability of hydrogen-like atoms

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Abstract. The Dirac Coulomb Green function in the representation of the annihilation and creation operators is established and on the basis of the application of this new operator representation an algebraic method of calculation of atomic characteristics is briefly discussed. The relativistic polarizability of hydrogen-like atoms is calculated and its simple analytical formula is obtained.

1. Introduction

The coordinate representation of the Coulomb Green function for the Dirac equation was first established by Martin and Glauber (1958) and has been used in the calculation of various problems in atomic and nuclear physics (see, for example, Zapryagaev *et al* 1985 and references therein). In concrete calculations some other different representations of this function are often used: the impulse representation (Gorshkov 1964, Manakov *et al* 1973), the coordinate representation in the expansion in power series of the Laguerre polynomial (Zon *et al* 1972, Zapryagaev and Manakov 1981).... However, the use of all the above-mentioned representations always leads to an enormous number of calculations of multi-dimensional integrals of special functions. This circumstance strongly decreases the efficiency of the application of analytical methods in perturbation theory with the use of the Dirac Coulomb Green function (in many papers this function is called the relativistic Coulomb Green function, see Swainson and Drake (1991)).

Currently the tendency to use the connection between the four-dimensional harmonic oscillator problem and the problem of a hydrogen atom in electromagnetic fields is intensively developing (see, for example, Komarov and Romanova 1982, Kibler and Negadi 1983, Le Van Hoang *et al* 1989). For relativistic Coulomb problems, a similar treatment was proposed in Komarov and Romanova (1985) and Le Van Hoang *et al* (1992) where, instead of the Dirac equation, an application was demonstrated of the equation in two-dimensional complex space (ξ-space), the set of solutions of which contains the solutions of the Dirac equation. The structure of the equation in ξ-space is simple in the sense that the equation term describing the interaction can be presented in the polynomial form of the coordinates and, therefore, is convenient for use in concrete algebraic calculations. In the

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present paper, on the basis of the equation suggested in Komarov and Romanova (1985), we establish the relativistic Coulomb Green function in the representation of the annihilation and creation operators; moreover this representation is established in such a way that all operators can be transformed into the normal form thereby allowing the use of the algebraic method of calculation. The use of an algebraic treatment does not need the explicit form of the wavefunctions, which enables us to reduce rather complicated calculations of the matrix elements with the Coulomb wavefunctions to a purely algebraic procedure of transforming the products of the creation and annihilation operators to a normal form (see Le Van Hoang *et al* 1989).

As a specific example of the application of the operator representation of the relativistic Coulomb Green function, we consider the problem of calculation of the static relativistic polarizability of hydrogen-like atoms, which has been the subject of many papers (Bartlett and Power 1969, Zon *et al* 1972, Labzowsky 1973, Barut and Nagel 1976, McDowell and Porter 1977, ...) and, in our view, is still of great interest for further research. We give in detail an analysis of and obtain a simple analytical formula for the relativistic polarizability in the ground state of hydrogen-like atoms with nuclear charge ranging from 1 to 137.

2. Equation in two-dimensional complex space

Let us consider the following equation:

$$\hat{H}\Psi(\xi) = Ze^2\Psi(\xi) \tag{1}$$

$$\hat{H} = -\tfrac{1}{2}\mathrm{i}\alpha_\lambda(\tau_\lambda)_{st}\left(\xi_t\frac{\partial}{\partial\xi_s} + \xi_s^*\frac{\partial}{\partial\xi_t^*}\right) + (m\beta - \varepsilon)\xi_s\xi_s^* \tag{2}$$

where the four-component spinor $\Psi(\xi)$ is a function of the complex coordinates ξ_s ($s = 1, 2$); α_λ ($\lambda = 1, 2, 3$) and β are Dirac matrices. Henceforth, we use the usual representation

$$\Psi = \begin{pmatrix}\Psi_1\\ \Psi_2\end{pmatrix} \qquad \alpha_\lambda = \begin{pmatrix}0 & \sigma_\lambda\\ \sigma_\lambda & 0\end{pmatrix} \qquad \beta = \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$$

where Ψ_1 and Ψ_2 are two-component spinors; σ_λ ($\lambda = 1, 2, 3$) are Pauli matrices. In the Hamiltonian (2) τ_λ ($\lambda = 1, 2, 3$) are Pauli matrices operating in the space of coordinates ξ, which are regarded as spinor components.

As shown in Komarov and Romanova (1985), after transformation into the usual three-dimensional space with the use of the correlations

$$x_\lambda = \xi_s^*(\tau_\lambda)_{st}\xi_t \qquad \chi = \arg(\xi_1) \tag{3}$$

equations (1) and (2) (for the class of wavefunctions, independent of the variable χ) lead to the Dirac equation for a charged particle with mass m and energy ε, moving in the Coulomb field $-Ze^2/r$. The existence of the above-mentioned connection allows us to use (1) and (2) in considering the relativistic Coulomb problems. For the problem of the motion of a Dirac particle in the Coulomb field plus an electromagnetic field $(\boldsymbol{A}, \varphi)$ we can use the following more generalized equation in ξ-space:

$$\left\{-\tfrac{1}{2}\mathrm{i}\alpha_\lambda(\tau_\lambda)_{st}\left(\xi_t\frac{\partial}{\partial\xi_s} + \xi_s^*\frac{\partial}{\partial\xi_t^*}\right) + (e\alpha_\lambda A_\lambda + m\beta + \varphi - \varepsilon)\xi_s\xi_s^* - Ze^2\right\}\Psi(\xi) = 0 \tag{4}$$

(see Le Van Hoang *et al* 1992). The condition of independence of the wavefunctions from the variable χ

$$-\mathrm{i}\frac{\partial}{\partial\chi}\Psi(\xi) = 0$$

can be rewritten as follows as an equation in ξ-space:

$$\hat{Q}\Psi(\xi) = 0 \tag{5}$$

where

$$\hat{Q} = \xi_s \frac{\partial}{\partial \xi_s} - \xi_s^* \frac{\partial}{\partial \xi_s^*} \,.$$

In concrete calculations, one usually needs equations for two-component spinors Ψ_1, Ψ_2 (quadratic Dirac equations). Therefore, we now establish the corresponding equations in ξ-space. By making the substitutions

$$\Psi_1 = \sqrt{m+\varepsilon}(\widetilde{F} + \widetilde{G}) \qquad \Psi_2 = \mathrm{i}\sqrt{m-\varepsilon}(\xi_u \xi_u^*)^{-1} \sigma_\lambda (\tau_\lambda)_{st} \xi_s^* \xi_t (\widetilde{F} - \widetilde{G}) \tag{6}$$

we transform (1) and (2), respectively, into the forms

$$\left(\xi_s \frac{\partial}{\partial \xi_s} + \xi_s^* \frac{\partial}{\partial \xi_s^*} + \omega \xi_s \xi_s^* - \frac{Ze^2 \varepsilon}{\omega}\right) \widetilde{F} - \left(1 + \sigma_\lambda \hat{l}_\lambda + \frac{Ze^2}{\omega}\right) \widetilde{G} = 0 \tag{7}$$

$$-\left(1 + \sigma_\lambda \hat{l}_\lambda - \frac{Ze^2}{\omega}\right) \widetilde{F} + \left(\xi_s \frac{\partial}{\partial \xi_s} + \xi_s^* \frac{\partial}{\partial \xi_s^*} - \omega \xi_s \xi_s^* + \frac{Ze^2 \varepsilon}{\omega}\right) \widetilde{G} = 0 \tag{8}$$

where $\omega = \sqrt{m^2 - \varepsilon^2}$ (henceforth, we consider the electron mass $m = 1$); $\hat{l}_\lambda$ is the orbital momentum operator, which in ξ-space has the form

$$\hat{l}_\lambda = -\tfrac{1}{2}(\tau_\lambda)_{st} \left(\xi_t \frac{\partial}{\partial \xi_s} - \xi_s^* \frac{\partial}{\partial \xi_t^*}\right) . \tag{9}$$

The fact that the operator $\hat{\kappa} = 1 + \sigma_\lambda \hat{l}_\lambda$ commutes with all operators occurring in (7) and (8) permits us to exclude one of the wavefunctions $\widetilde{F}$ and $\widetilde{G}$ from the equations, and as a result, obtain the following equations for each wavefunction:

$$\left\{\left(\xi_s \frac{\partial}{\partial \xi_s} + \xi_s^* \frac{\partial}{\partial \xi_s^*}\right)^2 - (\omega \xi_s \xi_s^*)^2 + (2Ze^2 \varepsilon + \omega) \xi_s \xi_s^* - \hat{\kappa}^2 + Z^2 e^4\right\} \widetilde{F} = 0 \tag{10}$$

$$\left\{\left(\xi_s \frac{\partial}{\partial \xi_s} + \xi_s^* \frac{\partial}{\partial \xi_s^*}\right)^2 - (\omega \xi_s \xi_s^*)^2 + (2Ze^2 \varepsilon - \omega) \xi_s \xi_s^* - \hat{\kappa}^2 + Z^2 e^4\right\} \widetilde{G} = 0 \,. \tag{11}$$

Equations (10) and (11) can be considered as having the quadratic form in ξ-space for the Dirac Coulomb particle. The scalar product of wavefunctions in ξ-space is defined by the following correlation:

$$(\widetilde{\Psi}|\widetilde{\varphi}) = \int \mathrm{d}^4\xi \, \widetilde{\Psi}^*(\xi_1', \xi_1'', \xi_2', \xi_2'') \, \widetilde{\varphi}(\xi_1', \xi_1'', \xi_2', \xi_2'') \tag{12}$$

where $\xi_s' \equiv \operatorname{Re} \xi_s, \xi_s'' \equiv \operatorname{Im} \xi_s$.

From (1) and (2) and (10) and (11) it is easy to see that the term which describes interaction in these equations is presented in a polynomial coordinate form. This circumstance allows us (in the next section) to establish algebraic solutions for the Coulomb problem, which serve as a convenient basis of wavefunctions for effective use in different calculations, in particular, for establishing a new operator representation of the relativistic Coulomb Green function.

3. Algebraic solutions of the Dirac equation for the Coulomb problem

The algebraic method for solving the Dirac equation for a charged particle in the Coulomb field was proposed by Komarov and Romanova (1985) on the basis of the application of (1) and (2). In this section, for further use, we develop this method and give the angular part of wavefunctions in general form.

Let us define operators

$$\begin{aligned} a_s &= \sqrt{\frac{\omega}{2}}\left(\xi_s + \frac{1}{\omega}\frac{\partial}{\partial \xi_s^*}\right) \qquad & b_s &= \sqrt{\frac{\omega}{2}}\left(\xi_s^* + \frac{1}{\omega}\frac{\partial}{\partial \xi_s}\right) \\ a_s^+ &= \sqrt{\frac{\omega}{2}}\left(\xi_s^* - \frac{1}{\omega}\frac{\partial}{\partial \xi_s}\right) \qquad & b_s^+ &= \sqrt{\frac{\omega}{2}}\left(\xi_s - \frac{1}{\omega}\frac{\partial}{\partial \xi_s^*}\right) \end{aligned} \tag{13}$$

where the parameter ω was defined in section 2. Operators (13) satisfy the commutation correlations

$$[a_s, a_t^+] = \delta_{st} \qquad [b_s, b_t^+] = \delta_{st} \tag{14}$$

(we have written only non-zero commutators). The possibility of using the algebraic method is conditioned by the fact that, all 'physical' operators can be expessed through the following 15 operators:

$$\begin{aligned} &M = a_s b_s \qquad && M^+ = a_s^+ b_s^+ \qquad && N = a_s^+ a_s + b_s^+ b_s \\ &m_\lambda = (\tau_\lambda)_{st} a_t b_s \qquad && m_\lambda^+ = (\tau_\lambda)_{st} a_s^+ b_t^+ && \\ &n_\lambda^a = (\tau_\lambda)_{st} a_s^+ a_t \qquad && n_\lambda^b = (\tau_\lambda)_{st} b_t^+ b_s && \end{aligned} \tag{15}$$

which form a closed algebra $SO(4,2)$ simply isomophic to the algebra of the group of dynamical symmetry of the system described by (1) and (2) (see Komarov and Romanova 1985). For example, in the representation (13)–(15) the operators occurring in (7), (8) and (10), (11) have the form

$$\begin{aligned} &\xi_s \frac{\partial}{\partial \xi_s} + \xi_s^* \frac{\partial}{\partial \xi_s^*} = M - M^+ - 2 \qquad && \xi_s \xi_s^* = \frac{1}{2\omega}(M + M^+ + N + 2) \\ &\hat{l}_\lambda = \tfrac{1}{2}(n_\lambda^a - n_\lambda^b) \qquad && x_\lambda = (\tau_\lambda)_{st} \xi_s^* \xi_t = \frac{1}{2\omega}(m_\lambda^+ + m_\lambda + n_\lambda^a + n_\lambda^b)\,. \end{aligned} \tag{16}$$

Let us now establish a basis of wavefunction vectors, which belong to a given value of the square of the orbital momentum l and a given value of its third projection m. Naturally, the basis wavefunction vectors have to belong to the zero eigenvalue of the operator $\hat{Q} = a_s^+ a_s - b_s^+ b_s$, i.e. they should be established through the vectors

$$(a_1^+)^{n_1} (a_2^+)^{n_2} (b_1^+)^{m_1} (b_2^+)^{m_2} |0(\omega)\rangle \tag{17}$$

where positive integers n_1, n_2, m_1, m_2 satisfy the correlation

$$n_1 + n_2 = m_1 + m_2\,. \tag{18}$$

$|0(\omega)\rangle$ is a vacuum state, defined by the equations

$$a_s |0(\omega)\rangle = b_s |0(\omega)\rangle = 0\,. \tag{19}$$

The operator of the third projection of orbital momentum $\hat{l}_3$ in the representation of operators (13)–(15) has the form

$$\hat{l}_3 = \tfrac{1}{2}(a_1^+ a_1 - a_2^+ a_2 - b_1^+ b_1 + b_2^+ b_2)$$

therefore, it is obvious to obtain the correlation

$$n_1 - n_2 - m_1 + m_2 = 2m \tag{20}$$

where m is a magnetic quantum number ($m = 0, \pm 1, \pm 2, \ldots$). Finally, taking into account the correlations (18) and (20), we find the wavefunction vector, which belongs to the given values of l and m in the form

$$|lm\rangle = \left(a_1^+ b_2^+\right)^{|m|} \sum_{k=0}^{N} C_k (a_1^+ b_1^+)^k (a_2^+ b_2^+)^{N-k} |0(\omega)\rangle \tag{21}$$

for $m > 0$ (for the case $m < 0$ the term $a_1^+ b_2^+$ should be replaced by $a_2^+ b_1^+$). Substituting (21) into the equation

$$\hat{L}^2 |lm\rangle = l(l+1)|lm\rangle$$

with the operator of the square of the orbital momentum has the form

$$\hat{L}^2 = \tfrac{1}{2} N(N+2) - M^+ M$$

and by using correlations (14) and (19), we obtain

$$|lm\rangle = (M^+)^j D_m^l (m^+) |0(\omega)\rangle \tag{22}$$

where

$$\begin{aligned} D_m^l (m^+)|0(\omega)\rangle = N_{lm} (a_1^+ b_2^+)^{|m|} \sum_{k=0}^{l-|m|} \frac{(-1)^k (l+|m|+k)!}{k!(k+|m|)!(l-|m|-k)!} (a_1^+ b_1^+)^k \\ \times (M^+)^{l-|m|-k} |0(\omega)\rangle \end{aligned} \tag{23}$$

and N_{lm} is a normalization constant. The existence of the operator $(M^+)^j$ in (22) is conditioned by the correlation

$$[\hat{L}^2, M^+] = 0$$

and is needed for constructing the radiation part of wavefunctions. The eigenvectors of operator $\hat{\kappa}$ can be established in the usual way from eigenvectors $\chi^{\uparrow(\downarrow)}$ of operator σ_3 and from vectors $D_m^l (m^+)|0(\omega)\rangle$. For further use, we establish some solutions $Z_{l\kappa}$,

$$\begin{aligned} Z_{1,2} &= \frac{1}{\sqrt{3}} \left(m_3^+ |0\rangle \chi^{\uparrow} - \tfrac{1}{2} (m_1^+ + \mathrm{i} m_2^+)|0\rangle \chi^{\downarrow} \right) \\ Z_{1,-1} &= \frac{1}{\sqrt{6}} \left(m_3^+ |0\rangle \chi^{\uparrow} + (m_1^+ + \mathrm{i} m_2^+)|0\rangle \chi^{\downarrow} \right). \end{aligned} \tag{24}$$

In section 4 we will use the basis vectors

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

for establishing wavefunctions and, therefore, it is neccessary to take note now of some correlations with respect to these basis vectors

$$\begin{aligned} M (M^+)^n Z_{l\kappa}(m^+)|0\rangle &= n(n+2l+1)(M^+)^{n-1} Z_{l\kappa}(m^+)|0\rangle \\ N (M^+)^n Z_{l\kappa}(m^+)|0\rangle &= 2(n+l)(M^+)^n Z_{l\kappa}(m^+)|0\rangle \end{aligned} \tag{25}$$

which are obtained by using (14) and (23).

4. Operator representation of the Dirac Coulomb Green function

The use of the method of perturbation theory to solve the Dirac equation for a charged particle moving in the Coulomb field plus an electromagnetic field, which is considered as a perturbation with respect to the first field, always leads to equations like (10) and (11), where a perturbative term exists in the right-hand side of the equations. In order to solve these equations there is a need to establish the corresponding Green functions. In the traditional coordinate treatment, these Green functions are called the Dirac Coulomb Green functions (see Martin and Glauber 1958, Zapryagaev *et al* 1985, Gorshkov 1964, Zon *et al* 1972, …). In our description, (10) and (11) have a structure which is convenient for establishing the Green operator through the annihilation and creation operators and for transforming this operator into a normal form.

Let us consider, for example, (10) and (11) with an inhomogeneous term on the right-hand side. In order to solve the above-mentioned equations we, first of all, have to exclude the existence of singularities appearing in places where $\xi_s\xi_s^* \to 0$ and expand the inhomogeneous term in power series of eigenvectors of the operators $\hat{L}^2$ and $\hat{\kappa}$. In this regard we represent wavefunctions in the form

$$\Phi = \sum_{l,\kappa} (\xi_s\xi_s^*)^\gamma \widetilde{\Phi}_{l\kappa}$$

where $\gamma = -l-1+\sqrt{\kappa^2 - Z^2e^4}$. Thus, the above-mentioned equations lead to the following equations for the wavefunctions $\widetilde{\Phi}_{l\kappa}$:

$$\left\{\left(\xi_s\frac{\partial}{\partial\xi_s} + \xi_s^*\frac{\partial}{\partial\xi_s^*} - 1 - l\right)^2 + 2(\gamma + l + 1)\left(\xi_s\frac{\partial}{\partial\xi_s} + \xi_s^*\frac{\partial}{\partial\xi_s^*} - 1 - l\right)\right.$$
$$\left. -(\omega\xi_s\xi_s^*)^2 + \left(2Ze^2\varepsilon \pm \omega\right)\xi_s\xi_s^*\right\}\widetilde{\Phi}_{l\kappa}(\xi) = \widetilde{\Phi}_{l\kappa}^{(o)}(\xi)\,. \qquad (26)$$

The operator in (26) can be rewritten in the form

$$\hat{H}_\pm = \tfrac{1}{4}(M - M^+ - 2l - 2)^2 + (\gamma + l + 1)(M - M^+ - 2l - 2)$$
$$-\tfrac{1}{4}(M + M^+ + N + 2)^2 + \alpha_\pm(M + M^+ + N + 2) \qquad (27)$$

where $\alpha_\pm = Ze^2\varepsilon/\omega \pm \frac{1}{2}$. Henceforth, for simplicity we leave out the signs ± in the description. By using the Green function operator $\hat{G}_{l\kappa}$ which satisfies the equation

$$\hat{G}_{l\kappa}\,\hat{H}\,\widetilde{\Phi}_{l\kappa}(\xi) = \widetilde{\Phi}_{l\kappa}(\xi) \qquad (28)$$

we establish the solution of (26) as follows:

$$\widetilde{\Phi}_{l\kappa}(\xi) = \hat{G}_{l\kappa}\widetilde{\Phi}_{l\kappa}^{(o)}(\xi)\,.$$

In order to establish $\hat{G}_{l\kappa}$ we turn to (28) and rewrite it in the overt form

$$\hat{G}_{l\kappa}\left\{\tfrac{1}{4}(M - M^+ - 2l - 2)^2 + (\gamma + l + 1)(M - M^+ - 2l - 2) - \tfrac{1}{4}(M + M^+ + N + 2)^2\right.$$
$$\left. + \alpha_\pm(M + M^+ + N + 2)\right\}(M^+)^n Z_{l\kappa}(m^+)|0\rangle = (M^+)^n Z_{l\kappa}(m^+)|0\rangle\,. \qquad (29)$$

By using correlations (25), equation (29) can be transformed into

$$\hat{G}_{l\kappa}(M + M^+ + N + 2)\left\{-\left(n + \gamma + l + \tfrac{3}{2} - \alpha_\pm\right)(M^+)^n - (2\gamma + 1)(-1)^n n!\right.$$
$$\left.\sum_{k=0}^{n-1}\frac{(-1)^k}{k!}(M^+)^k\right\}Z_{l\kappa}(m^+)|0\rangle = (M^+)^n Z_{l\kappa}(m^+)|0\rangle \qquad (30)$$

which suggests that the operator $\hat{G}_{l\kappa}$ should be found in the form

$$\hat{G}_{l\kappa} = \hat{B}_{l\kappa}\frac{1}{2+N+M+M^{+}} \qquad \hat{B}_{l\kappa} = \sum_{s=0}^{\infty} d_s(N/2)M^s \tag{31}$$

where $d_s(N/2)$ are functions with argument $N/2$. Further, we substitute (31) into (30), use correlations (25) in the action of operators and consider all the coefficients with the same vectors to be equal to zero. Consequently, we obtain the following system of algebraic equations for $d_s(N/2)$:

$$\begin{aligned}
&-\left(n+\gamma+l+\tfrac{3}{2}-\alpha_{\pm}\right)d_0(n+l) = 1\\
&(-1)^s\left(n+\gamma+l+\tfrac{3}{2}-\alpha_{\pm}\right)(n+2l+1)!d_s(n-m+l)\\
&\qquad +(2\gamma+1)\sum_{t=0}^{s-1}(-1)^t(t+n-s+2l+1)!\,d_t(n-s+l) = 0 \qquad s=1,2,\ldots.
\end{aligned} \tag{32}$$

By solving the system of equations (32) with respect to unknown functions $d_s(n+l)$ we obtain

$$\begin{aligned}
d_0(n) &= -\frac{1}{n+\gamma+\frac{3}{2}-\alpha_{\pm}}\\
d_s(n) &= (-1)^s(2\gamma+1)\frac{(n+l+1)!}{(n+s+l+1)!}\,\frac{\Gamma\left(n+s-\gamma+\frac{1}{2}-\alpha_{\pm}\right)\Gamma\left(n+\gamma+\frac{3}{2}-\alpha_{\pm}\right)}{\Gamma\left(n-\gamma+\frac{3}{2}-\alpha_{\pm}\right)\Gamma\left(n+s+\gamma+\frac{5}{2}-\alpha_{\pm}\right)}.
\end{aligned} \tag{33}$$

As a result, the Green function operator is finally established in a normal form

$$\begin{aligned}
\hat{B}_{l\kappa} = \frac{1}{\frac{1}{2}N+\gamma+\frac{3}{2}-\alpha_{\pm}}\Bigg[-1+(2\gamma+1)\sum_{s=1}^{\infty}(-1)^s\frac{\left(\frac{1}{2}N+l+1\right)!}{\left(\frac{1}{2}N+s+l+1\right)!}\\
\times\frac{\Gamma\left(\frac{1}{2}N+s-\gamma+\frac{1}{2}-\alpha_{\pm}\right)\Gamma\left(\frac{1}{2}N+\gamma+\frac{5}{2}-\alpha_{\pm}\right)}{\Gamma\left(\frac{1}{2}N-\gamma+\frac{3}{2}-\alpha_{\pm}\right)\Gamma\left(\frac{1}{2}N+s+\gamma+\frac{5}{2}-\alpha_{\pm}\right)}M^s\Bigg].
\end{aligned} \tag{34}$$

The operator representation of the Green function (34) allows us in concrete calculations to reduce rather complicated calculations of matrix elements into purely algebraic operations like (25). In the next section we will demonstrate such algebraic calculations through the exemplary problem of relativistic hydrogen-like atoms in a homogeneous electric field.

5. Relativistic polarizability of hydrogen-like atoms

Let us now consider the Dirac equation for an electron with energy ε_e, moving in the Coulomb field of the nucleus with charge Ze and in the external homogeneous electric field E. After transformation into ξ-space and after the substitution of (6) the Dirac equation leads to the following equations:

$$\begin{aligned}
&\left(x_\lambda\frac{\partial}{\partial x_\lambda}+1+\omega_e r-\frac{Ze^2\varepsilon_e}{\omega_e}\right)\widetilde{F}-\left(\hat{\kappa}+\frac{Ze^2}{\omega_e}\right)\widetilde{G} = -\frac{eE}{\omega_e}rx_3(\varepsilon_e\widetilde{F}+\widetilde{G})\\
&\left(\hat{\kappa}-\frac{Ze^2}{\omega_e}\right)\widetilde{F}+\left(x_\lambda\frac{\partial}{\partial x_\lambda}+1-\omega_e r+\frac{Ze^2\varepsilon_e}{\omega_e}\right)\widetilde{G} = \frac{eE}{\omega_e}rx_3(\widetilde{F}+\varepsilon_e\widetilde{G})
\end{aligned} \tag{35}$$

where $\omega_{\mathrm{e}} = \sqrt{1-\varepsilon_{\mathrm{e}}^2}$. Here and henceforth, all operators in (35) will be interpreted as operators in ξ-space corresponding to the formal changes

$$\begin{aligned}
&r \to \xi_s \xi_s^* \qquad x_\lambda \to (\tau_\lambda)_{st} \xi_s^* \xi_t \\
&x_\lambda \frac{\partial}{\partial x_\lambda} \to \frac{1}{2}\left(\xi_s \frac{\partial}{\partial \xi_s} + \xi_s^* \frac{\partial}{\partial \xi_s^*}\right) \\
&\hat{l}_\lambda \to -\tfrac{1}{2}(\tau_\lambda)_{st}\left(\xi_t \frac{\partial}{\partial \xi_s} - \xi_s^* \frac{\partial}{\partial \xi_t^*}\right) .
\end{aligned} \tag{36}$$

Equations (35) will be solved using the method of perturbation theory with respect to the external electric field. Considering the dimensionless value of the strength of the electric field E as a small parameter we expand the wavefunctions $\widetilde{F}$ and $\widetilde{G}$ in power series of this parameter

$$\begin{aligned}
\widetilde{F} &= \widetilde{F}^{(0)} + E\widetilde{F}^{(1)} + E^2\widetilde{F}^{(2)} + \cdots \\
\widetilde{G} &= \widetilde{G}^{(0)} + E\widetilde{G}^{(1)} + E^2\widetilde{G}^{(2)} + \cdots .
\end{aligned} \tag{37}$$

By the expansion (37), ε_{e} and ω_{e} for the ground state can be expressed as follows:

$$\varepsilon_{\mathrm{e}} = \varepsilon - \tfrac{1}{2}aE^2 + \cdots \qquad \omega_{\mathrm{e}} = \omega + \frac{a\varepsilon}{2\omega}E^2 + \cdots \tag{38}$$

where a is defined as the polarizability of the hydrogen-like atoms. Here in (38), we take into account the well known fact that the linear Stark effect is absent for the ground state. By substituting (37) and (38) into (35), and considering to be zero all the coefficients with the same order of the parameter E, we obtain for every order of approximation the equations for wavefunctions $\widetilde{F}^{(k)}$, $\widetilde{G}^{(k)}$.

The formula for the ground state polarizability can thus be obtained

$$a = -\frac{2\omega e}{\varepsilon}\left(\langle \widetilde{F}^{(0)}|rx_3|\widetilde{F}^{(1)}\rangle - \varepsilon\langle \widetilde{F}^{(0)}|rx_3|\widetilde{G}^{(1)}\rangle\right) . \tag{39}$$

The wavefunctions in the zero-order approximation $\widetilde{F}^{(0)}$ and $\widetilde{G}^{(0)}$ which, in fact, are solutions of equations like (10) and (11), can be established by using the algebraic method (see Komarov and Romanova 1985). We obtain

$$\widetilde{F}^{(0)} = \frac{1}{(2\omega)^{1-\varepsilon}\sqrt{\Gamma(2\varepsilon)}} r^{\varepsilon-1}|0(\omega)\rangle\chi^{\uparrow} \qquad \widetilde{G}^{(0)} = 0 \tag{40}$$

where $\omega = Ze^2$, $\varepsilon = \sqrt{1-Z^2e^4}$. Then, in equations for wavefunctions in the first-order approximation, the perturbation has the form

$$\begin{aligned}
\frac{erx_3}{\omega}(\varepsilon\widetilde{F}^{(0)} + \widetilde{G}^{(0)}) &= \frac{2e\varepsilon}{(2\omega)^{1-\varepsilon}\sqrt{\Gamma(2\varepsilon)}} r^{\varepsilon} m_3^{+}|0(\omega)\rangle\chi^{\uparrow} \\
&= v_\varepsilon \varepsilon r^{\varepsilon}(\sqrt{2}\, Z_{1,2} + Z_{1,-1})
\end{aligned} \tag{41}$$

where

$$v_\varepsilon = \frac{2\sqrt{6}\, e(2\omega)^{\varepsilon-3}}{3\sqrt{\Gamma(2\varepsilon)}} .$$

It can easily be seen from (41) that $\widetilde{F}^{(1)}$ and $\widetilde{G}^{(1)}$ can be represented as follows:

$$\widetilde{F}^{(1)} = \widetilde{F}_{+}^{(1)} + \widetilde{F}_{-}^{(1)} \qquad \widetilde{G}^{(1)} = \widetilde{G}_{+}^{(1)} + \widetilde{G}_{-}^{(1)} \tag{42}$$

where $\widetilde{F}_{\pm}^{(1)}$ and $\widetilde{G}_{\pm}^{(1)}$ are defined by the equations

$$\begin{aligned}
&\left(x_\lambda \frac{\partial}{\partial x_\lambda} + 1 + \omega r - \frac{Ze^2\varepsilon}{\omega}\right) \widetilde{F}_{-}^{(1)} = -\varepsilon v_\varepsilon r^\varepsilon Z_{1,-1} \\
&\left(x_\lambda \frac{\partial}{\partial x_\lambda} + 1 - \omega r + \frac{Ze^2\varepsilon}{\omega}\right) \widetilde{G}_{-}^{(1)} - 2\widetilde{F}_{-}^{(1)} = -v_\varepsilon r^\varepsilon Z_{1,-1}
\end{aligned} \tag{43}$$

and

$$\begin{aligned}
&\left(x_\lambda \frac{\partial}{\partial x_\lambda} + 1 + \omega r - \frac{Ze^2\varepsilon}{\omega}\right) \widetilde{F}_{+}^{(1)} + 3\widetilde{G}_{+}^{(1)} = -\sqrt{2}\,\varepsilon v_\varepsilon r^\varepsilon Z_{1,2} \\
&\left(x_\lambda \frac{\partial}{\partial x_\lambda} + 1 - \omega r + \frac{Ze^2\varepsilon}{\omega}\right) \widetilde{G}_{+}^{(1)} + \widetilde{F}_{+}^{(1)} = -\sqrt{2}\,\varepsilon v_\varepsilon r^\varepsilon Z_{1,2}\,.
\end{aligned} \tag{44}$$

In a simple way the solutions of (43) can be obtained in a form

$$\begin{aligned}
\widetilde{F}_{-}^{(1)} &= \tfrac{1}{2}\varepsilon v_\varepsilon r^{\varepsilon-2}\left[\frac{2(\varepsilon+1)(2\varepsilon+1)}{(2\omega)^3} - r^2\right] Z_{1,-1} \\
\widetilde{G}_{-}^{(1)} &= -\frac{1+\varepsilon}{2\omega} v_\varepsilon r^{\varepsilon-2}\left[r + \frac{2\varepsilon+1}{(2\omega)}\right] Z_{1,-1}\,.
\end{aligned} \tag{45}$$

The system of equations (44) is more complicated in comparison with (43) and, therefore, for its solution the Green function should be used. As a result, we obtain

$$\begin{aligned}
\widetilde{F}_{+}^{(1)} &= \left(M^{+} + \tfrac{1}{2}N + 1 - \varepsilon\right)\widetilde{G}_{+}^{(1)} - \sqrt{2} v_\varepsilon r^\varepsilon Z_{1,2} \\
\widetilde{G}_{+}^{(1)} &= \sqrt{2}(2-\varepsilon) v_\varepsilon r^\gamma \hat{G}_{12}\, r^{-\gamma+\varepsilon} Z_{1,2}\,.
\end{aligned} \tag{46}$$

Substituting $\widetilde{F}^{(1)}$ and $\widetilde{G}^{(1)}$ into (39) and by using (25) as well as the correlation

$$r^n Z_{l\kappa} = \frac{(2\omega)^{-n}}{\Gamma(-n)} \sum_{s=0}^{\infty} \frac{(-1)^s}{s!} \frac{\Gamma(s-n)\Gamma(2+2l+n)}{\Gamma(s+2+2l)} (M^{+})^s Z_{l\kappa} \tag{47}$$

we finally obtain the formula for the polarizability

$$a = a_0 + \delta \tag{48}$$

with

$$\begin{aligned}
a_0 &= \frac{e^2(\varepsilon+1)(2\varepsilon+1)(4\varepsilon^2+13\varepsilon+12)}{36\omega^4} - \frac{e^2(\varepsilon-2)^2\Gamma(\varepsilon+\gamma+4)\,\Gamma(3+\varepsilon-\gamma)}{216(\gamma-\varepsilon+3)\,\Gamma(2\varepsilon)\,\varepsilon\omega^4} \\
\delta &= -\frac{e^2(\varepsilon-2)^2\Gamma(\varepsilon+\gamma+4)\,\Gamma(3+\varepsilon-\gamma)}{36\varepsilon\omega^4\Gamma(2\varepsilon)\,\Gamma(-\varepsilon-\gamma)\,\Gamma(-\varepsilon+\gamma+1)} \times \left(\sum_{k=1}^{\infty} \frac{\Gamma(k-\varepsilon-\gamma)\,\Gamma(k-\varepsilon+\gamma+1)}{k!\,(k+3)!\,(k+\gamma-\varepsilon+3)}\right. \\
&\qquad -(2\gamma+1)\sum_{q=1}^{\infty} \frac{\Gamma(q-\varepsilon+\gamma+1)\,\Gamma(q-\varepsilon-\gamma+2)}{(q+3)!\,\Gamma(q-\varepsilon+\gamma+4)} \\
&\qquad \left.\times \sum_{s=0}^{q-1} \frac{\Gamma(s-\varepsilon-\gamma)\,\Gamma(s-\varepsilon+\gamma+3)}{s!\,\Gamma(s-\varepsilon-\gamma+3)}\right)
\end{aligned}$$

where $\gamma = -2 + \sqrt{4 - Z^2 e^4}$.

The numerical values of a and a_0 for Z ranging from 1 to 137 are given in table 1. The corresponding graph describing the dependence of the polarizability on nuclear charge Z is also given (see figure 1). Taking into account the fact that $Ze^2 < 1$ for $Z \leqslant 137$ we expand a in a power series of Ze^2

$$a = \frac{9e^2}{2(Ze^2)^4}\left[1 - \frac{28}{27}(Ze^2)^2 + \frac{2\pi^2+31}{432}(Ze^2)^4 + \cdots\right]. \tag{49}$$

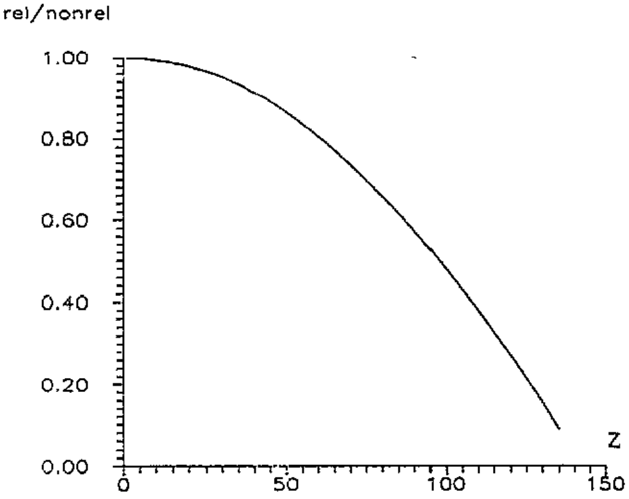

Figure 1. The dependence of the polarizability on nuclear charge Z.

Table 1. Relativistic polarizability in the ground state of hydrogen-like atoms; a, a_{non} are the relativistic and non-relativistic polarizabilities respectively; $a_{\text{non}} = 9e^2/2(Ze^2)^{-4}$; a_0 is an analytical estimation term of a.

Z	a/a_{non}	a_0/a_{non}	Z	a/a_{non}	a_0/a_{non}
1	0.999 945	0.999 945	40	0.912 499	0.912 099
2	0.999 779	0.999 778	45	0.889 547	0.889 039
3	0.999 503	0.999 501	50	0.864 040	0.863 412
4	0.999 117	0.999 113	55	0.836 027	0.835 265
5	0.998 620	0.998 613	60	0.805 562	0.804 655
6	0.998 012	0.998 004	65	0.772 707	0.771 642
7	0.997 295	0.997 283	70	0.737 526	0.736 294
8	0.996 467	0.996 451	75	0.700 091	0.698 683
9	0.995 529	0.995 509	80	0.660 478	0.658 887
10	0.994 481	0.994 456	85	0.618 769	0.616 993
11	0.993 323	0.993 292	90	0.575 049	0.573 088
12	0.992 055	0.992 019	95	0.529 404	0.527 267
13	0.990 677	0.990 635	100	0.481 922	0.479 623
14	0.989 189	0.989 141	105	0.432 680	0.430 250
15	0.987 592	0.987 536	110	0.381 741	0.379 222
16	0.985 885	0.985 821	115	0.329 122	0.326 582
17	0.984 068	0.983 997	120	0.274 744	0.272 283
18	0.982 143	0.982 062	125	0.218 279	0.216 049
19	0.980 108	0.980 018	130	0.158 625	0.156 872
20	0.977 964	0.977 865	135	0.090 429	0.089 657
25	0.965 616	0.965 461	136	0.073 004	0.072 582
30	0.950 569	0.950 345	137	0.045 002	0.045 236
35	0.932 853	0.932 547			

The numerical data of a (see table 1) and the expansion (49) coincide with results given in Zon *et al* (1972). But in our results, it should be noted that the series appearing in δ are quickly convergent and the value δ/a_0 for all values of Z is very small. The biggest value, whereby $Z = 130$, is $\delta/a_0 \sim 0.01$. This result allows us to use a_0 as a simple analytical formula for the polarizability of the ground state of hydrogen-like atoms. In fact, it is useful for analysis of different effects connected with the problem of interaction of two hydrogen-like atoms having high values of nuclear charge (see Baras 1988). Furthermore, we consider it interesting and useful to scale the polarizability with various size parameters. The size of hydrogen-like atom could be defined as follows:

$$\tilde{r} = \int \mathrm{d}^3\boldsymbol{r}\, |\Psi(\boldsymbol{r})|^2\, r\,.$$

For the ground state of hydrogen-like atoms, we have

$$\tilde{r} = \frac{\langle \widetilde{F}^{(0)} | r^2 | \widetilde{F}^{(0)} \rangle}{\langle \widetilde{F}^{(0)} | r | \widetilde{F}^{(0)} \rangle} = \frac{2\sqrt{1 - Z^2e^4} + 1}{2Ze^2}$$

from which it follows that

$$\tilde{r}^4 \simeq 5.06\left(1 - \tfrac{4}{3}\left(Ze^2\right)^2 + \tfrac{1}{3}\left(Ze^2\right)^4 + \cdots\right)\frac{1}{\left(Ze^2\right)^4}\,. \tag{50}$$

The comparison of (49) with (50) leads to the conclusion that the relativistic polarizability scales like $\tilde{r}^4$ for low values of nuclear charge.

It should be noted that the high convergency of the power series appearing in the expression for δ as well as the high accuracy of the analytical estimation a_0 are directly related to the expansion (34) of the Dirac Coulomb Green function. This expansion in the coordinate representation leads to power series of the oscillator wavefunctions. The results obtained serve as a good example for demonstrating the advantage of the latter in comparison with the use of the usual representations which lead to power series of the Coulomb wavefunctions. In our next work, we will show the above-mentioned efficiency in calculations of the dynamical relativistic polarizability of hydrogen-like atoms, a problem which is rarely investigated because of its complexity.

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