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DIRAC-COULOMB PROBLEM IN THE SECOND-ORDER DIRAC EQUATION APPROACH

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The detailed analysis of the relativistic Coulomb problem is presented on the basis of the second-order Dirac equation. For an electron in the Coulomb potential of a pointlike nucleous, the different sets of fundamental solutions are investigated both for linear and squared Dirac equations. A number of representations are discussed for the relativistic Coulomb Green's function and wavefunctions of bound and continuum states. The explicit form of the reduced Coulomb Green's function is presented for an arbitrary bound state of the relativistic electron. The Sturmian expansions of Green's function for linear and squared Dirac equations are especially analysed. The advantages of the second-order Dirac equation approach are demonstrated to connect all known analytical results for both, relativistic and nonrelativistic Coulomb Green functions and wavefunctions. It is shown that all results for the linear Coulomb-Dirac equation follow from the simple algebra by the second-order Dirac equation solution.

1. Introduction

An impressive progress, achieved in the last decade in quantum electrodynamics calculations of multicharged ion energy levels (see Mohr *et al* 1998 and references cited herein), was caused mostly by developing the Furry representation methods (Furry 1951, Schweber 1961). In this approach the perturbation theory on both, electron-electron and electron-vacuum interactions is developed on the basis of the complete set of electron states in an atomic potential V. In many cases the Coulomb potential of a pointlike nucleus with the atomic number Z is a good approximation. An analysis of various expressions for the Coulomb wavefunctions, and especially for the Coulomb Green function, is the important problem, because these objects are the basis of the quantum electrodynamics calculations in the relativistic theory of multicharged ions and heavy atoms (see, e. g., Zapriagaev *et al* 1985, Labzowsky *et al* 1993, Borovskii *et al* 1995).

In contrast to the free electron case, the momentum representation for the electron's propagator in an external field depends upon the momentum **p** and **p**′ separately, but does not only from the momentum transfer $\mathbf{p} - \mathbf{p}'$. In this reason, the momentum representation is inefficient in quantum electrodynamics of the bound states, and the coordinate representation for propagators is more convenient. At present time the closed form of the relativistic Coulomb Green function G_E is unknown, therefore the partial expansions of $G_E(\mathbf{r}, \mathbf{r}')$ in terms of the states with definite total angular momentum j, its projection m and parity p=± 1 are used.

Apparently, the Dirac-Coulomb Green function $G_E(\mathbf{r}, \mathbf{r}')$ in quantum electrodynamics calculations was used first by Wichmann and Kroll (1956). In this work the regular method to construct the fundamental set of solutions for Dirac-Coulomb equation was used. The kind of these solutions was similar to the standard one offered by Gordon (1927). The complicated dependence of $G_E(\mathbf{r}, \mathbf{r}')$ on the radial variables r and r' by means of Whittaker functions of variables $r_>$ and $r_<$ [$r_>$ ($r_<$) is larger (smaller) of r and r'] didn't enable to apply it widely in analytical calculations. Martin and Glauber (1958) suggested the other approach to take into account the Coulomb field in virtual states of a relativistic electron - the method of the Green function for the second-order (or squared) Dirac equation, $\mathcal{G}_E(E; \mathbf{r},\mathbf{r}')$ (see (27) below). In this approach the Dirac-Coulomb Green function $G_E(\mathbf{r},\mathbf{r}')$ is obtained from $\mathcal{G}_E(\mathbf{r},\mathbf{r}')$ as a result of the action of a linear differential operator $\hat{\mathbf{K}}$ (so-called «squared operator») on $\mathcal{G}_E(\mathbf{r},\mathbf{r}')$. Hostler (1964) has performed a general analysis of the Coulomb Green function theory and employed a special integral representation for the product of Whittaker functions to receive the explicit expression for the radial part of $\mathcal{G}_E(\mathbf{r},\mathbf{r}')$, symmetric in r and r'. The function $\mathcal{G}_E(\mathbf{r},\mathbf{r}')$ was used successfully by Brown et al (1974) to study some problems of the vacuum polarization by a strong Coulomb field. At the same time, Mohr (1974) has carried out first the nonperturbative in (αZ) [α is the fine structure constant] numerical calculation of the selfenergy correction $\sim\alpha$ for hydrogenlike (H-) ions using the Coulomb Green function $G_E(\mathbf{r},\mathbf{r}')$. This function was studied in details performing the exact calculations of vacuum polarization effects in a strong Coulomb field (Manakov *et al* 1989, Fainshtein *et al* 1990). Swainson and Drake (1991) obtained another form of $G_E(\mathbf{r},\mathbf{r}')$ using a special linear transformation for the solutions of Dirac equation. This form of G_E was used particularly for the recalculation of Mohr (1974) result with higher accuracy (Pachucki, 1993).

Besides the quantum electrodynamics applications, the formalism of relativistic Coulomb Green functions has an important role in the relativistic quantum mechanics of atomic systems. To make the analytical calculation of atomic parameters it is preferable to write Green functions in a symmetric form with respect to variables r and r'. The well-known expansion of nonrelativistic Coulomb Green function in terms of the so-called Sturmian functions (Hostler, 1970) is an example of such a symmetric form for the Green function. The radial part of Sturmian functions is expressed in terms of the Laguerre polynomials. The complete sets of these polynomials, both for the relativistic and nonrelativistic cases, were introduced by Fock (1932), who pointed out the usefulness of these set of functions for the Coulomb problem. The symmetric form of $\mathcal{G}_E(\mathbf{r},\mathbf{r}')$ similar to the nonrelativistic Hostler result was derived for the first time by Zon *et al* (1972) on the basis of bilinear generating function for the Laguerre polynomials (see also Granovski and Nechet 1974). This method was used also by Swainson and Drake (1991). The relativistic Sturmian functions were introduced first by Manakov *et al* (1973) together with the Sturmian expansion of $\mathcal{G}_E(\mathbf{r},\mathbf{r}')$ obtained by the direct solution of the differential equation for $\mathcal{G}_E(\mathbf{r},\mathbf{r}')$. Later, the expansions of $G_E(\mathbf{r},\mathbf{r}')$ in terms of series involved the products of Laguerre polynomials were obtained both for regular form of G_E involving Whittaker functions (Zapriagaev and Manakov 1981) and by direct acting of the squared operator $\hat{\mathbf{K}}$ on $\mathcal{G}_E(\mathbf{r},\mathbf{r}')$ (Zapriagaev and Manakov 1976). Recently, slightly modified comparing with dissused above, expansions of $G_E(\mathbf{r},\mathbf{r}')$ in terms of Sturmian functions for the squared Dirac equation (Manakov *et al* 1973) were published (Szymanowski *et al* 1997a, Szmytkowski 1997, 1998, Manakov and Zapriagaev 1997).

The Sturmian-like expansions of $\mathcal{G}_E$ and G_E have allowed to receive a number of particular analytical results for the ions with high Z (see, e. g., Zapriagaev *et al* 1985). The DC electric and magnetic field atomic susceptibilities and shielding factors of H-like ions (Manakov *al* 1974), the lowest order correlation correction to the atomic parameters of He-like ions (Zapriagaev *et al* 1979,1982) *e.t.c.* were among them. Besides analytical calculations, Sturmian expansions of $\mathcal{G}_E$ are effective also in numerical calculations of relativistic two-photon transitions with the exact account of retardation effects (see, e. g., Manakov *et al* 1987, Szymanovski *et al* 1997b).

In the present work the complete analysis is given for the Dirac-Coulomb problem based only on the second-order Dirac equation. In other words the direct solution of the linear Dirac equation is not used at all. Particularly, in the developed approach the results have the most close form to the nonrelativistic one. Namely, the regular and irregular solutions of the Dirac equation are the linear combinations of two Whittaker functions, as in the traditional form (Gordon, 1927; Wichman and Kroll, 1956), but in this case they have other parameters. As a result, for the bound-state wavefunction, a combination of two Laguerre polynomials arises, one of which vanishes in the nonrelativistic limit and the other one gives the nonrelativistic wavefunction. The continuum-state wavefunctions have also an obvious advantage in this approach, e. g., well-known free-electron wavefunctions are obtained naturally in the limit Z=0. In the second-order Dirac equation approach such a structure of Dirac-Coulomb equation solution is evident, because the nonrelativistic limit follows from the second-order Dirac equation in the most elegant way (Schweber 1963). The mentioned form of the Dirac-Coulomb equation solution may be especially useful for its αZ power series expansions. The similar structure of Dirac-Coulomb wavefunctions was received earlier by a number of authors (see Wong and Hisn-Yang Yeh 1982, Zapriagaev 1987, Swainson and Drake 1991). Nevertheless, a detailed analysis of the Coulomb problem (including the sets of fundamental solutions, Green functions, *e.t.c.*) on the basis of the squared Dirac equation was not performed and that is the major goal of the present paper. A brief description of key results of this analysis was published recently (Manakov and Zapriagaev 1997).

The paper is organized as follows: In Sec. 2 a brief review of the second-order Dirac equation problem is presented. The regular and irregular solutions of Dirac-Coulomb equation are presented in Sec. 3 in terms of the squared Dirac equation solutions. In Sec. 4 various representations of the Dirac-Coulomb Green function are derived. The relativistic wavefunctions of bound and continuum states together with their nonrelativistic limits are discussed in Sec. 5. The expressions for the reduced Dirac-Coulomb Green function are presented in Sec. 6.

2. Review of the second-order Dirac-Coulomb equation

2.1 Regular and irregular solutions. Sturmian functions

The Dirac equation for the stationary states of electron in the Coulomb field of the point charge Ze is

$$\hat{D}(E;\mathbf{r})\Psi(E;\mathbf{r})\equiv\left[c(\gamma\cdot\hat{\mathbf{p}})+m_ec^2+\gamma^0\left(-\frac{Ze^2}{r}-E\right)\right]\Psi(E;\mathbf{r})=0. \tag{1}$$

Here γ^0,γ are the Dirac matrices: $\gamma^0=\beta=\begin{pmatrix} I & 0\\ 0 & -I\end{pmatrix}$,

$\gamma=\beta\alpha=\begin{pmatrix} 0 & \sigma\\ -\sigma & 0\end{pmatrix}$, where σ and I denote 2 by 2 Pauli, and the unit matrix, respectively, E is the electron energy, m_e is the electron mass. The operator $\hat{D}(E;\mathbf{r})$ is connected with the Dirac-Coulomb Hamiltonian $\hat{H}$ by the relation of $\hat{D}(E;\mathbf{r})=\beta(\hat{H}-E)$, where $\hat{H}=c(\alpha\cdot\mathbf{p})+\beta m_ec^2-Ze^2/r$.

In the second-order Dirac equation approach a new function, $\Phi(E;r)$, is introduced, instead of Ψ, by the relation

$$\Psi(E;r)=\hat{\mathbf{K}}\Phi(E;r). \tag{2}$$

Here $\hat{\mathbf{K}}$ is the dimensionless, so-called «squared operator», which differs from the operator $\hat{D}(E;\mathbf{r})$ by opposite sign of the electron mass m_e:

$$\hat{\mathbf{K}}=-\frac{1}{2m_ec^2}\left[c(\gamma\cdot\hat{\mathbf{p}})-m_ec^2+\gamma^0\left(-\frac{Ze^2}{r}-E\right)\right]. \tag{3}$$

The substitution of (2) into (1), after the standard transformations with γ-matrices, leads to the second-order Dirac equation, which may be written in the form suggested by Martin and Glauber (1958)

$$\left[\frac{\hbar^2}{2m_e}\left(\frac{1}{r}\frac{\partial^2}{\partial r^2}r-\frac{\hat{\mathcal{L}}(\hat{\mathcal{L}}+1)}{r^2}\right)+\frac{Ze^2}{r}\frac{E}{m_ec^2}+\frac{E^2-m_e^2c^4}{2m_ec^2}\right]\Phi(E;r)=0. \tag{4}$$

Here $\hat{\mathcal{L}}=\hat{\mathcal{K}}-i\alpha Z(\alpha\cdot\mathbf{n})$ is the spin-angular operator (so-called «Johnson's operator»), which includes the well-known Dirac operator $\hat{\mathcal{K}}=-(\sigma\cdot\mathbf{l})/\hbar-1$. $\mathbf{n}=\mathbf{r}/r$, $\hat{\mathbf{l}}=[\mathbf{r}\times\hat{\mathbf{p}}]$ is the orbital momentum operator, $\alpha=e^2/\hbar c$ is the fine structure constant. Note, that $\hat{\mathcal{L}}$ is non-Hermitian operator, but $\beta\hat{\mathcal{L}}$ is a Hermitian one. It is important that operator

$$\hat{\Lambda}=\hat{\mathcal{L}}(\hat{\mathcal{L}}+1)=\hat{\Lambda}=\hat{\mathbf{l}}^2/\hbar^2-i\alpha Z(\alpha\cdot\mathbf{n})-(\alpha Z)^2$$

involves all matrix structure of the second-order Dirac equation (4). After the substitution $\hat{\Lambda}\to\mathbf{l}^2/\hbar^2$ the equation (4) coincides with the Schrödinger equation for the nonrelativistic Kepler problem. So, the second-order Dirac equation approach is the most straightforward way to receive the nonrelativistic limit in the Dirac-Coulomb problem.

We shall discuss below briefly the solution of (4) with definite values of total angular momentum $\mathbf{j}$ and its projection $j_z=m\hbar$. The general structure of this solution was discussed in a number of works (see, e. g., Martin and Glauber 1958, Biedenharn 1962, Hostler 1964, Brown *et al* 1971, Zon *et al* 1972).

Let $k=\pm 1, \pm 2$ ... be the eigenvalues of operator $\hat{\mathcal{K}}$. It is more convenient to present k as $k=s\,\kappa$, where $\kappa=|k|$ and s = sign(k)=± 1. The total angular momentum $\hat{\mathbf{j}}=\hat{\mathbf{l}}+\hbar\sigma/2$ and the orbital momentum operators are connected with the Dirac operator $\hat{\mathcal{K}}$ by the relations $\hat{\mathbf{j}}^2=\hbar^2(\hat{\mathcal{K}}^2-1/4)$, $\mathbf{l}^2=\hbar^2\hat{\mathcal{K}}(\hat{\mathcal{K}}+1)$. Thus, for fixed k, the quantum numbers j and l are $j=j(k)=\kappa-1/2$, $l=l(k)=\kappa+(s-1)/2$. Due to the anticommutation between $\hat{\mathcal{K}}$ and $(\sigma\cdot\mathbf{n})$, there is no commutation of $\hat{\mathcal{K}}$ with $\hat{\mathcal{L}}$. On the other hand, due to the anticommutation between $(\alpha\cdot\mathbf{n})$ and operators $\hat{\mathcal{K}}$ and β, the operator $\hat{\mathrm{K}}=-\beta\hat{\mathcal{K}}$ commutes with $\hat{\mathcal{L}}$. Moreover, it is clear from the above definitions that $[\hat{j}_z,(\sigma\cdot\mathbf{n})]=[\hat{j}_z,\hat{\mathcal{K}}]=[\hat{j}_z,\hat{\mathcal{L}}]=0$. Thus, the Jhonson's operator $\hat{\mathcal{L}}$ commutes with $\hat{\mathrm{K}},\hat{j}^2,\hat{j}_z$ and the eigenfunctions Θ of these operators can be constructed using the well-known complete set of eigenfunctions for Dirac operator $\hat{\mathcal{K}}$:

$$\hat{\mathcal{K}}\chi_m^k = k\chi_m^k(\mathbf{n}),\quad \chi_m^k(\mathbf{n}) = \sum_{m_1,m_2} C_{l(k)\ m_1\ 1/2 m_2}^{j(k)\ m} Y_{l(k)m_1}(\mathbf{n})u_{m_2} \tag{5}$$

where u_m is an eigenfunction of the electron spin operator $\hbar\sigma/2$, Y_{lm} is the spherical harmonic and $C_{b\ \beta\ c\ \gamma}^{a\ \alpha}$ is the Clebsch-Gordon coefficient.

Martin and Glauber (1958) and Biedenharn (1962) derived the spin-angular part, $\Theta(\mathbf{n})$, of the function $\Phi(E;\mathbf{r})$ in (4) with fixed j and m in an operator form. In our notations their result is

$$\Theta_{km}^{(q)}(\mathbf{n}) = \hat{\mathcal{S}}\chi_m^{k,q}(\mathbf{n}),$$
$$\hat{\mathcal{S}} = \cosh(\vartheta/2) - i(\alpha\cdot\mathbf{n})\sinh(\vartheta/2), \tag{6}$$

where $\vartheta = \tanh^{-1}(\alpha Z/\hat{\mathcal{K}})$, and $\chi_m^{k,q}$ are the eigenfunctions of operators $\hat{\mathcal{K}}$ (see (5)), $\hat{j}_z$ and of the matrix β simultaneously:

$$\chi_m^{k,+1} = \begin{pmatrix}\chi_m^k\\ 0\end{pmatrix},\quad \chi_m^{k,-1} = \begin{pmatrix}0\\ \chi_m^k\end{pmatrix}. \tag{7}$$

Obviously, the eigenvalues of β-matrix on a class of functions (7) are q=±1. Because functions (7) are the eigenfunctions of the operator $\hat{\mathcal{K}}$ with eigenvalues $k = s\kappa$, the substitution $\hat{\mathcal{K}} = k$ in the operator $\hat{\mathcal{S}}$ in (6) leads to the equivalent form of $\Theta_{km}^{(q)}$:

$$\Theta_{km}^{(q)}(\mathbf{n}) = \hat{\mathcal{S}}(k)\chi_m^{k,q}(\mathbf{n}),$$
$$\hat{\mathcal{S}}(k) = \sqrt{\frac{\kappa+\lambda}{2\lambda}}\left[1 - is\frac{\alpha Z}{\kappa+\lambda}(\alpha\cdot\mathbf{n})\right], \tag{8}$$

where $\hat{\mathcal{S}}(k)$ is an operator in the subspace of functions with the definite k. The parameter λ in (8) is: $\lambda = \sqrt{\kappa^2 - (\alpha Z)^2}$.

The functions $\Theta_{km}^{(q)}(\mathbf{n})$ are the eigenfunctions of operator $\hat{\mathcal{L}}$ with two different eigenvalues $\mathcal{L}_s = s\lambda$ and each of them is twofold degenerate in the sign(q)=± 1. The orthonormalization condition of these functions is

$$< \overline{\Theta_{k,m}^{(q)}}\,|\Theta_{k',m'}^{(q')} >= q\ \ \delta_{q,q'}\ \ \delta_{k,k'}\ \ \delta_{m,m'}, \tag{9}$$

where $\overline{\Theta} = \Theta^{+}\beta$. The functions $\Theta_{k,m}^{(q)}$ form the complete set in the spin-angular space

$$\sum_{k=-\infty}^{\infty}\sum_{m=-\kappa}^{\kappa}\sum_{q=\pm1} q\Theta_{k,m}^{(q)}(\mathbf{n})\overline{\Theta_{k,m}^{(q)}(\mathbf{n}')} = \delta(\mathbf{n}-\mathbf{n}').$$

The additional factor q in these expressions appears as the consequence of identities following from (8)

$$\beta\hat{\mathcal{S}}^{+}(k)\beta = \hat{\mathcal{S}}(k),\quad \overline{\Theta_{k,m}^{(q)}} = \Theta_{k,m}^{(q)+}\beta = \left(\chi_m^{k,q}\right)^{+}\hat{\mathcal{S}}(k). \tag{10}$$

The same identity as for $\hat{\mathcal{S}}$ can be obtained for the operator $\hat{\mathcal{L}}$, namely $\beta\hat{\mathcal{L}}^{+} = \hat{\mathcal{L}}\beta$.

Obviously, the functions $\Theta(\mathbf{n})$ can be derived also as the solution of the eigenvalue problem for non-Hermitian operator $\hat{\mathcal{L}}$:

$$\hat{\mathcal{L}}\theta = \mathcal{L}\theta. \tag{11}$$

Choosing θ as the eigenfunctions of operator $\hat{\mathrm{K}} = -\beta\hat{\mathcal{K}}$ (since $[\hat{\mathcal{L}},\hat{\mathcal{K}}] = 0$), we present the equation (11) in the following matrix form

$$\theta = \begin{pmatrix} a(k)\chi_m^k\\ b(k)\chi_m^{-k}\end{pmatrix},$$

$$\begin{pmatrix}\hat{\mathcal{K}} & -i\alpha Z(\sigma\cdot\mathbf{n})\\ -i\alpha Z(\sigma\cdot\mathbf{n}) & \hat{\mathcal{K}}\end{pmatrix}\begin{pmatrix}a\chi_m^k\\ b\chi_m^{-k}\end{pmatrix} = \mathcal{L}\begin{pmatrix}a\chi_m^k\\ b\chi_m^{-k}\end{pmatrix}.$$

The last equation yields the secular equation for the coefficients $a(k)$, $b(k)$ and eigenvalues $\mathcal{L}$:

$$\begin{cases} a(k-\mathcal{L}) + i\alpha Z\, b = 0\\ i\alpha Z\, a - (k+\mathcal{L})b = 0.\end{cases} \tag{12}$$

Two different eigenvalues of operator $\hat{\mathcal{L}}$ can be found from (12): $\mathcal{L}_p = p\lambda$, where $p = \pm1$. So, four different eigenfunctions of $\hat{\mathcal{L}}$ exist at fixed κ and m, and we may write the most general form for these functions:

$$\theta_{1,k,m} = c_1\begin{pmatrix}\sqrt{\kappa+\lambda}\,\chi_m^k\\ i\sqrt{\kappa-\lambda}\,\chi_m^{-k}\end{pmatrix},\quad \theta_{3,k,m} = c_3\begin{pmatrix}\sqrt{\kappa+\lambda}\,\chi_m^{-k}\\ -i\sqrt{\kappa-\lambda}\,\chi_m^{k}\end{pmatrix},$$

$$\theta_{2,k,m} = c_2\begin{pmatrix}i\sqrt{\kappa-\lambda}\,\chi_m^{-k}\\ \sqrt{\kappa+\lambda}\,\chi_m^{k}\end{pmatrix},\quad \theta_{4,k,m} = c_4\begin{pmatrix}-i\sqrt{\kappa-\lambda}\,\chi_m^{k}\\ \sqrt{\kappa+\lambda}\,\chi_m^{-k}\end{pmatrix}, \tag{13}$$

where c_i are normalization constants. The orthogonality between these functions follows from (11). It is easy to verify by direct calculations that the functions $\theta_i(\mathbf{n})$ are orthogonal only with matrix β, and the orthonormalization condition is (see (9))

$$< \overline{\theta_{\tau',\kappa'\ m'}}\,|\theta_{\tau,\kappa m} >= (-1)^{\tau+1}\delta_{\tau,\tau'}\delta_{\kappa,\kappa'}\delta_{m,m'},$$

where the coefficients c_τ in (13) are equal to $e^{i\alpha_\tau}/\sqrt{2\lambda}$, and $\mathrm{Im}\,\alpha_\tau = 0$. Note, that the factor $(-1)^{\tau+1}$ in the orthonormalization condition for θ_i does no problem in our case because we deal with eigenfunctions of non-Hermitian operator (see (10)). If we use the sign (k) and the additional index $p = \pm 1$ to label the four functions (13) with the fixed phase factors $e^{i\alpha_\tau}$, they may be written in compact form. If $\alpha_\tau = 0$ these functions are

$$\Theta_{k,m}^{(p)} = \frac{1}{\sqrt{2\lambda}}\begin{pmatrix}(is)^{\frac{1-p}{2}}\sqrt{\kappa+p\lambda}\,\chi_m^{kp}\\ (is)^{\frac{1+p}{2}}\sqrt{\kappa-p\lambda}\,\chi_m^{-kp}\end{pmatrix},$$

and they are identical to (8) as follows immediately from (8) using the trivial relation $(\alpha\cdot\mathbf{n})\chi_m^{k,p}(\mathbf{n}) = -\chi_m^{-k,-p}(\mathbf{n})$. We will use below the eigenfunctions of $\hat{\mathcal{L}}$ in more convenient way for the applications form

$$\theta_{k,m}^{(p)} = \frac{1}{\sqrt{2\lambda}}\begin{pmatrix}\sqrt{\kappa+p\lambda}\,\chi_m^{kp}\\ ips\sqrt{\kappa-p\lambda}\,\chi_m^{-kp}\end{pmatrix} = \sqrt{\frac{\kappa+p\lambda}{2\lambda}}\begin{pmatrix}\chi_m^{kp}\\ is\dfrac{\alpha Z}{\kappa p+\lambda}\chi_m^{-kp}\end{pmatrix}. \tag{14}$$

These functions coincide with (8) by the relation $\theta_{k,m}^{(p)} = e^{i\pi s(p-1)/4}\Theta_{k,m}^{(p)}$. Note, that in our notations the functions $\theta_{k,m}^{(p)}$ are the eigenfunctions of operator $\hat{K}$ with eigenvalues $K = sp\kappa = kp$, but not $K = s\kappa$ as for the $\Theta_{k,m}^{(p)}$ - functions.

For the operators $\hat{\mathcal{L}}$ and $\hat{\Lambda} = \hat{\mathcal{L}}(\hat{\mathcal{L}}+1)$ we have $\hat{\mathcal{L}}\theta_{k,m}^{(p)} = s\lambda\theta_{k,m}^{(p)}$, $\hat{\Lambda}\theta_{k,m}^{(p)} = \lambda(\lambda+s)\theta_{k,m}^{(p)}$. Thus, the general solution of equation (4) with definite value of p, $K = kp$ and m may be written as:

$$\Phi_{k,m}^{(p)}(E;r) = \frac{1}{x}\varphi_k(\varepsilon;x)\theta_{k,m}^{(p)}(\mathbf{n}). \tag{15}$$

where the radial functions $\varphi_k(\varepsilon;x)$ satisfy the standard Whittaker equation

$$\left[\frac{d^2}{dx^2} - \frac{1}{4} + \frac{\eta}{x} - \frac{\lambda(\lambda+s)}{x^2}\right]\varphi_k(\varepsilon;x) = 0. \tag{16}$$

Here and below, we use the dimensionless units, which are natural for relativistic Coulomb problem $\varepsilon = E/m_ec^2$, $\nu = \alpha/\sqrt{1-\varepsilon^2}$, $\eta = \varepsilon\nu Z$, $x = 2r/\nu a_0$, $a_0 = \hbar^2/m_ec^2$ is the Bohr radius.

As a fundamental system of solutions for the equation (16) we choose the following Whittaker functions (Erdelyi *et al* 1953a)

$$\varphi_k^r(\varepsilon;x) = M_{\eta,\lambda+s/2}(x),\quad \varphi_k^{ir}(\varepsilon;x) = W_{\eta,\lambda+s/2}(x),$$

which lead to the regular (Φ^r) or irregular (Φ^{ir}) at origin solutions of equation (4) in the gap region $-m_ec^2 < E < m_ec^2$. The point $x = 0$ is the branch point for the Whittaker functions, so they are determined as the single-valued analytical functions of x in a complex x-plane with the cut along the interval $(-\infty,0]$ of real x-axis, i. e. at $|\arg x| \le \pi$. Since $x = 2r\sqrt{1-\varepsilon^2}/\alpha a_0$, for a finite r our solutions $\varphi_k^r(\varepsilon;x)$ and $\varphi_k^{ir}(\varepsilon;x)$ are analytical functions of the energy $E = m_ec^2\varepsilon$ in the complex E-plane with the branch cuts along the intervals $(-\infty, m_ec^2]$ and $[m_ec^2,\infty)$ of the real axis. We define the square root $\sqrt{1-\varepsilon^2}$ as positive in the interval $-m_ec^2 < E < m_ec^2$ of the real E-axis. Out this interval we fix the sign of the square root by the condition $\mathrm{Re}\left(\sqrt{1-\varepsilon^2}\right) \ge 0$, which determines the «physical sheet» of the two-sheeted Riemann surface for this square root (see, Landau and Lifshitz (1977)). So, going over the branch cut $E > m_ec^2$ from the interval $-m_ec^2 < E < m_ec^2$ in the upper complex half-plane E we have $\sqrt{1-\varepsilon^2} \to -i\sqrt{\varepsilon^2-1}$, and therefore the parameters ν, η, x for the positive continuum are

$$\nu \to i\alpha\frac{m_ec}{p},\ \eta \to i\xi,\ x \to -i2pr/\hbar, \tag{17}$$

where $p = m_ec\sqrt{\varepsilon^2-1}$, $\xi = \alpha Z\varepsilon/\sqrt{\varepsilon^2-1}$. Instead of functions M and W, the other form of the radial part of (15) is more preferable for the continuum solutions φ^r, φ^{ir}, namely

$$\frac{1}{x}\varphi_k^r(\varepsilon;x) = \frac{1}{x}M_{i\xi,\lambda+s/2}\left(-2i\frac{p}{\hbar}r\right) =$$
$$= \frac{\Gamma(2\lambda+2\delta_s)}{\Gamma(\lambda+\delta_s-i\xi)}\exp\left(-\frac{\pi}{2}\xi - i\Delta_k\right)F_k(\varepsilon;r), \tag{18}$$

$$\frac{1}{x}\varphi_k^{ir}(\varepsilon;x)=\frac{1}{x}W_{i\xi,\lambda+s/2}\left(-2i\frac{p}{\hbar}r\right)=i\exp\left(\frac{\pi}{2}\xi+i\Delta_k\right)G_k^{(+)}(\varepsilon;r)=$$

$$=i\exp\left(\frac{\pi}{2}\xi+i\Delta_k\right)\left[G_k^{(-)}(\varepsilon;r)+iF_k(\varepsilon;r)\right].$$

Here $\Delta_k(\varepsilon)=\arg\Gamma(\lambda+\delta_s+i\xi)+\frac{\pi}{2}(\lambda+\delta_s-1)$; $\delta_s=(s+1)/2$; $F_k(\varepsilon;r)$ and $G_k^{(\pm)}(\varepsilon;r)$ are the regular and irregular continuum wavefunctions with the following asymptotic behaviour at $r\to\infty$

$$F_k(\varepsilon;r)=\frac{\hbar}{pr}\sin\left\{\frac{p}{\hbar}r+\xi\ln\left(2\frac{p}{\hbar}r\right)-\Delta_k\right\}$$

$$G_k^{(\pm)}(\varepsilon;r)=\frac{\hbar}{2pr}\exp\left\{\pm i\frac{p}{\hbar}r+\xi\ln\left(2\frac{p}{\hbar}r\right)-\Delta_k\right\}. \quad (19)$$

So, the choice of the signs (17) generates the irregular solutions with the asymptotic form of divergent spherical waves at $r\to\infty$. Evidently, the opposite signs lead to the convergent-wave solution. These functions are similar completely to the well-known nonrelativistic regular and irregular Coulomb solutions $F_l(p;r)$ and $G_l^{(\pm)}(\varepsilon;r)$ with an orbital momentum l and $p=\sqrt{2m_eE}$. The above discussion will be useful also below to investigate the analytical structure of Green functions and fundamental solutions for the linear Dirac equation.

Obviously, the bound-state energies, $E_i=m_ec^2\varepsilon_i$, are the same both for second-order and linear Dirac equations and they are determined by the condition

$$\lambda+\delta_s-\eta(\varepsilon_i)\equiv\lambda+(s+1)/2-\frac{\varepsilon_i\alpha Z}{\sqrt{1-\varepsilon_i^2}}=-n_i, \quad (20)$$

$n_i=0,1,2,...$

In this case the Whittaker functions are the bound solutions of equation (16) in accordance with the following identities for the Whittaker functions $M_{\alpha,\beta}$, $W_{\alpha,\beta}$ (Gradshtein and Ryzhik 1967)

$$\frac{(-1)^{n_i}}{n_i!}W_{\bar{\eta}_i,\lambda+s/2}(x)=\frac{\Gamma(n_i+2\lambda+2\delta_s)}{n_i!\,\Gamma(2\lambda+2\delta_s)}M_{\bar{\eta}_i,\lambda+s/2}(x)=$$

$$=x^{\lambda+\delta_s}\exp(-x/2)L_{n_i}^{2\lambda+s}(x). \quad (21)$$

Here $\Gamma(x)$ is the Gamma-function, $L_n^{\alpha}(x)$ is the Laguerre polynomial, $\bar{\eta}_i=n_i+\lambda+\delta_s$, $n_i=0,1,2,...$. If the radial quantum number, n_r is defined by the following relation

$$n_r\equiv n_i+\delta_s=n_i+(s+1)/2=\begin{cases}0,1,2,..., & at\ k=-\kappa,\\ 1,2,3,..., & at\ k=\kappa\end{cases},$$

the equation (20) gives the well-known expression for the Dirac-Coulomb energy eigenvalues

$$\varepsilon_{nk}=1\Big/\sqrt{1+\frac{\alpha Z^2}{(n_r+\lambda)^2}}=\frac{\gamma}{N},\quad \gamma=n_r+\lambda=\sqrt{N^2-\alpha Z^2},$$

$$N=\sqrt{n^2-2n_r(\kappa-\lambda)}. \quad (22)$$

Here $n=n_r+\kappa$ is the principal quantum number, $n=1,2,3,...$. So, the energy is two-fold degenerated in the sign of k, exception the case of $n_r=0$ which is achieved only at $s=-1$, i. e. at $k=-n$. The corresponding radial bound-state wavefunctions are expressed in the terms of Laguerre polynomials as it is evident from (21).

Besides the above-mentioned solutions of the second-order Dirac equation (4), the so-called Sturmian functions of this equation are useful for different applications too. The Sturmian function is the solution of equation (4) where the replacement $Z\to\sigma Z$ is made, with σ the eigenvalue of the equation. These functions have the spin-angular structure of equation (15):

$$S_{nkm}^{(p)}(E;r)=\frac{1}{x}\phi_{nk}\left(\frac{2r}{\nu a_0}\right)\theta_{k,m}^{(p)}(\mathbf{n}), \quad (23)$$

but the radial functions ϕ_{nk} are the solutions of the Sturm-Liouville problem for the following equation (cf. with (16))

$$\left[\frac{d^2}{dx^2}-\frac{1}{4}+\sigma_n\frac{\eta}{x}-\frac{\lambda(\lambda+s)}{x^2}\right]\phi_{nk}(x)=0.$$

The bound solutions of this equation at $|E|<mc^2(|\varepsilon|<1)$ have the form

$$\phi_{nk}=\sqrt{\frac{n!}{\Gamma(n+2\lambda+2\delta_s)}}\,x^{\lambda+\delta_s}exp\left(-\frac{x}{2}\right)L_n^{2\lambda+s}(x),$$

$$\sigma_n=n+\lambda+\delta_s-1,\ n=0,1,... \quad (24)$$

The Sturmian functions (24) are orthonormalized by the condition

$$\int_0^\infty\phi_{nk}(x)\frac{1}{x}\phi_{n'k}(x)dx=\delta_{n,n'}$$

and they form a complete set of functions with a discrete spectrum only.

We mention that the similar functions both for the relativistic and the nonrelativistic Coulomb problem were introduced by Fock (1932). But only after Rotenberg (1962) the nonrelativistic Sturmian functions are widely used as the convenient basis set in the calculations of different atomic problems (see, e.g., (Manakov *et al* 1986) and the recent review by Maquet *et al* (1998)). The Sturmian set for the second-order Dirac equation was introduced by Manakov *et al* (1973).

2.2 The Green function of the second-order Dirac equation

The Dirac-Coulomb Green function $G_E(\mathbf{r},\mathbf{r}')$ is defined as the solution of the differential equation (see eq.(1))

$$\hat{D}(E;\mathbf{r})G_E(\mathbf{r},\mathbf{r}')=\delta(\mathbf{r}-\mathbf{r}'). \quad (25)$$

Similarly to (2) we shall express $G_E(\mathbf{r},\mathbf{r}')$ in terms of the second-order Dirac equation Green function $\mathcal{G}_E(\mathbf{r},\mathbf{r}')$ by the relation

$$G_E(\mathbf{r},\mathbf{r}')=\hat{\mathbf{K}}\mathcal{G}(E;\mathbf{r},\mathbf{r}'). \quad (26)$$

The Green function $\mathcal{G}_E(\mathbf{r},\mathbf{r}')$ satisfies the following equation

$$\left[\frac{\hbar^2}{2m_e}\left(\frac{1}{r}\frac{\partial^2}{\partial r^2}r-\frac{\hat{\mathcal{L}}(\hat{\mathcal{L}}+1)}{r^2}\right)+\frac{Ze^2}{r}\frac{E}{m_ec^2}+\right.$$

$$\left.+\frac{E^2-m_e^2c^4}{2m_ec^2}\right]\mathcal{G}(E;\mathbf{r},\mathbf{r}')=-\delta(\mathbf{r}-\mathbf{r}'),$$

The partial-wave expansion of $\mathcal{G}_E(E;\mathbf{r},\mathbf{r}')$ is

$$\mathcal{G}(E;\mathbf{r},\mathbf{r}')=\sum_k g_k(E;r,r')\sum_{m,p}p\,\theta_{k,m}^{(p)}(\mathbf{n})\overline{\theta_{k,m}^{(p)}(\mathbf{n}')}, \quad (27)$$

where the radial part g_k satisfies the equation

$$\left[\frac{\hbar^2}{2m_e}\left(\frac{1}{r}\frac{\partial^2}{\partial r^2}r-\frac{\lambda(\lambda+s)}{r^2}\right)+\frac{Ze^2}{r}\frac{E}{m_ec^2}+\right.$$

$$\left.+\frac{E^2-m_e^2c^4}{2m_ec^2}\right]g_k(E;r,r')=-\frac{\delta(r-r')}{rr'}.$$

Here we use the notations which were introduced in the previous Section. The solution of this equation may be written in a standard form as a product of the regular and irregular solutions of (16) divided on the Wronskian of these solutions

$$g_k(E;r,r')=\frac{4m_e}{\hbar^2a_0\nu}\frac{\Gamma(\lambda-\eta+\delta_s)}{\Gamma(2\lambda+2\delta_s)}\frac{1}{xx'}M_{\eta,\lambda+s/2}(x_<)W_{\eta,\lambda+s/2}(x_<) \quad (28)$$

The variables $x_>$ and $x_<$ are: $x_>=\max(x,x')$, $x_<=\min(x,x')$, $x=2r/\nu a_0$. Note that the result (28) was obtained also by Hostler (1964) by the direct calculation of the integral over the continuum in the spectral expansion of g_k in terms of the bound- and continuum-state solutions of radial equation (16).

We suppose, that the energy E in equation (28) lies in the interval $-m_ec^2<E<m_ec^2$. For the energies outside this region we should fix the boundary conditions for $g_k(E;r,r')$. The choice of signs (17) generates from (28) the Green function with the divergent wave asymptotic behavior (cf. (18))

$$g_k^{(+)}(E;r,r')=-\frac{4m_ep}{\hbar^3}F_k(\varepsilon;r_<)G_k^{(+)}(\varepsilon;r_>)=$$

$$=-\frac{4m_ep}{\hbar^3}\left[F_k(\varepsilon;r_<)G_k^{(-)}(\varepsilon;r_>)+iF_k(\varepsilon;r)F_k(\varepsilon;r')\right]. \quad (29)$$

Since $G_k^{(-)}(\varepsilon;r)=G_k^{(+)*}(\varepsilon;r)$, the Green function $g_k^{(-)}(E;r,r')$ is complex-conjugate to (29) in conformity with opposite signs in (17). So it is clear, that a simple relation between $g_k^{(\pm)}(E;r,r')$ exists

$$g_k^{(-)}(E;r,r')-g_k^{(+)}(E;r,r')=i\frac{8m_ep}{\hbar}F_k(\varepsilon;r)F_k(\varepsilon;r'). \quad (30)$$

Finally note, that

$$g_k^{(0)}(E;r,r')=\frac{1}{2}\left[g_k^{(-)}(E;r,r')+g_k^{(+)}(E;r,r')\right]$$

is the Green function with the standing-wave asymptotic form which is used, e. g., in the R-matrix approach of the collision theory (Newton 1967).

The expressions (28), (29) for g_k with variables $x_>$, $x_<$ are quite standard. Hostler (1964) has presented them in the form symmetric by x and x' with the use of a special integral representation for the product of Whittaker functions with different arguments:

$$g_k(E;r,r')=\frac{4m_e}{\hbar^2 a_0 \nu\sqrt{xx'}}\times$$

$$\times\int_0^1 \frac{t^{-\eta-1/2}}{1-t}\exp\left(-\frac{x+x'}{2}\frac{1+t}{1-t}\right)I_{2\lambda+s}\left(\frac{2\sqrt{xx't}}{1-t}\right)dt \quad (31)$$

Here $I_p(z)$ is the modified Bessel function of the first kind. The integral (31) exists if $\mathrm{Re}\,\eta<\lambda+(s-1)/2$ and in opposite case it may be transformed to the contour integral by the substitution

$$\int_0^1 dt\, t^{-\eta} f(t)=\frac{1}{\exp(-i2\pi\eta)-1}\oint_1^{(0+)} z^{-\eta} f(z)dz.$$

The symmetric expansion of $g_k(E;r,r')$ in terms of the Laguerre polynomial series was derived by Zon *et al* (1972) using the bilinear generating function for the Laguerre polynomials (so-called Hille-Hardy formula (Erdelyi *et al* 1953b):

$$g_k(E;r,r')=\frac{4m_e}{\hbar^2 a_0\nu}(xx')^{\lambda+\delta_s-1}\exp\left(-\frac{x+x'}{2}\right)\times$$

$$\times\sum_{n=0}^{\infty}\frac{n!L_n^{2\lambda+s}(x)L_n^{2\lambda+s}(x')}{\Gamma(n+2\lambda+2\delta_s)(n-\eta+\lambda+\delta_s)}. \quad (32)$$

The simplest method to derive the result (32) is an expansion of $\mathcal{G}_E(\mathbf{r},\mathbf{r}')$ in a series of Sturmian functions (23). This approach used by Manakov *et al* (1973) gives:

$$\mathcal{G}(E;\mathbf{r},\mathbf{r}')=\frac{4m_e}{\hbar^2 a_0\nu}\sum_{nkmp} p\frac{S_{nkm}^{(p)}(E;\mathbf{r})\overline{S_{nkm}^{(p)}(E;\mathbf{r}')}}{n-\eta+\lambda+\delta_s}. \quad (33)$$

Note that the expansions (32), (33) are less general then the symmetric representation (31), because the series in n of these expansions converge only if $|E|<m_e c^2$. But they also may be used in analytical calculations for arbitrary energies E if the resulting formulae may be analytically continued. The generalization of (32) for the numerical calculations at $|E|>m_e c^2$ was derived by Manakov *et al* (1984) on the basis of a special re-expansion of $L_n^{2\lambda+s}(x)$ into the series of Laguerre polynomials $L_m^{2\lambda+s}(zx)$ with an arbitrary (complex) parameter z.

So, the results of this Section yield all necessary information on the Coulomb problem in the second-order Dirac equation approach. For small αZ we have $\lambda+(s-1)/2=\lambda-\kappa+l\approx l-(\alpha Z)^2/2\kappa+\ldots$, and after the substitution of $\lambda+(s-1)/2=l$ the radial equation (16) coincides with the radial Schrödinger equation for the Coulomb problem. Therefore in this case all the above-discussed results are transformed immediately to the corresponding nonrelativistic expressions. Particularly, the well-known Sturmian expansion of the nonrelativistic Coulomb Green function (Hostler 1970) follows from (33).

3. Regular and irregular solutions of linear Dirac equation

Accordingly to the general theory of motion in the central field, the solution of equation (1) with the fixed total angular momentum $j=\kappa-1/2$, its projection m on the z-axis and the parity $(-1)^{j+s/2}$ has the following general form

$$\Psi_{k,m}(E;\mathbf{r})=\frac{1}{r}\begin{pmatrix} f_{+1}(E;r)\chi_m^{k} \\ if_{-1}(E;r)\chi_m^{-k}\end{pmatrix}, \quad (34)$$

where radial parts $f_{\pm1}$ of large and small components of a wavefunction in the Coulomb field satisfy the linear system of differential equations:

$$\frac{df_p}{d\rho}+p\frac{k}{\rho}f_p-p\left(\varepsilon+p+\frac{\alpha Z}{\rho}\right)f_{-p}=0,\quad p=\pm1, \quad (35)$$

where $\rho=r\,m_e c/\hbar$, $\varepsilon=E/m_e c^2$, k is an eigenvalue of Dirac operator $\hat{\mathcal{K}}$.

Gordon (1928) and Darvin (1928) suggested to solve the system (35) for the bound and continuum wavefunctions by the substitution $f_{\pm1}\sim\sqrt{1\pm\varepsilon}(u_1\pm u_2)$. As a result, the new functions, u_1 and u_2, are expressed in terms of Whittaker functions, and a regular $(\Psi_{k,m}^{r})$ and an irregular $(\Psi_{k,m}^{ir})$ in origin solutions of Dirac equation are presented as combinations of two Whittaker functions, namely

$$f_p^r(E;x)=\frac{\sqrt{1+p\varepsilon}}{x^{1/2}}\left[(\lambda-\eta)M_{\eta-1/2,\lambda}(x)+\right.$$

$$\left.+p(Z\nu-k)M_{\eta+1/2,\lambda}(x)\right],$$

$$f_p^{ir}(E;x)=\frac{\sqrt{1+p\varepsilon}}{x^{1/2}}\left[(Z\nu+k)W_{\eta-1/2,\lambda}(x)+pW_{\eta+1/2,\lambda}(x)\right] \quad (36)$$

The notations introduced in Sec. 2 are used here, $\lambda=\sqrt{\kappa^2-(\alpha Z)^2}$, $\nu=\alpha/\sqrt{1-\varepsilon^2}$, $\eta=\nu Z\varepsilon$, $x=2r/\nu a_0$. A solution of the Dirac equation (1) in the form (34), (36) we call below as the standard form of a Dirac equation solution. Certainly, the sign choice (17) should be used in (36) for the continuum states with the divergent wave asymptotic behavior.

Now we shell consider the connection of solutions (34), (36) with the solutions of the second-order Dirac equation. As (4) is the second-order equation, it has the number of solutions twice the number of solutions of the (linear) Dirac equation (1), at the same E, j, m and parity. So the solutions of (4) have an additional index p. On the other hand, each solution of the second-order Dirac equation generates the appropriate solution of linear equation in the accordance with the relation (2). Thus, one can expect that (i) the linear combinations of pairs of solution $\Phi_{k',m}^{(p)}$ with fixed k' and different p or with fixed p but different $s'=\mathrm{sign}(k')$ give the same solution $\Psi_{k,m}$, or (ii) few different solutions $\Phi_{k',m}^{(p)}$ with different p, k' lead to the same solution $\Psi_{k,m}$. Evidently, in the last case different forms can represent the same solution of eq. (1). We will show that just the case (ii) is realized.

Expressing the squared operator $\hat{\mathbf{K}}$ in dimensionless units with separate radial and angular variables

$$\hat{\mathbf{K}}=\sqrt{1-\varepsilon^2}\left[i(\gamma\cdot\mathbf{n})\left(\frac{1}{x}\frac{\partial}{\partial x}x+\frac{\hat{\mathcal{L}}}{x}\right)+\frac{1+\beta\varepsilon}{2\sqrt{1-\varepsilon^2}}\right], \quad (37)$$

it is easy to calculate the action of operator $\hat{\mathbf{K}}$ on the arbitrary solution of the second-order Dirac equation in form (15) of any type (regular or irregular one). After some algebra this result may be written as follows

$$\hat{\mathbf{K}}\Phi_{k,m}^{(p)}(E;\mathbf{r})=\frac{1}{2\lambda x}\sqrt{\frac{\kappa+p\lambda}{2\lambda}}\times$$

$$\times\begin{pmatrix}\left[\lambda+\varepsilon\kappa p+s\alpha Z\frac{\sqrt{1-\varepsilon^2}}{\kappa p+\lambda}\hat{D}(k;x)\right]\phi_k(\varepsilon;x)\chi_m^{kp}(\mathbf{n}) \\ i\left[s\alpha Z\frac{\lambda+\varepsilon\kappa p}{\kappa p+\lambda}+\sqrt{1-\varepsilon^2}\hat{D}(k;x)\right]\phi_k(\varepsilon;x)\chi_m^{-kp}(\mathbf{n})\end{pmatrix}, \quad (38)$$

where $\hat{D}(k;x)$ is the linear differential operator

$$\hat{D}(k;x)=2\lambda\left(\frac{d}{dx}+s\frac{\lambda}{x}-s\frac{\eta}{2\lambda}\right),$$

and ϕ_k is the radial part of an arbitrary solution of equation (16) similar to (15).

The expression (38) may be written in a more simple matrix form

$$\hat{\mathbf{K}}\Phi_{k,m}^{(p)}(E;\mathbf{r})=\frac{\lambda+\varepsilon\kappa p}{2\lambda x}\hat{S}^{(p)}(k)\begin{pmatrix}\phi_k(\varepsilon;x)\chi_m^{kp}(\mathbf{n}) \\ i\frac{\sqrt{1-\varepsilon^2}}{\lambda+\varepsilon\kappa p}\hat{D}(k;x)\phi_k(\varepsilon;x)\chi_m^{-kp}(\mathbf{n})\end{pmatrix} \quad (39)$$

introducing the matrix operator

$$\hat{S}^{(p)}(k)=\sqrt{\frac{\kappa+p\lambda}{2\lambda}}\left[1+is\frac{\alpha Z}{\kappa p+\lambda}(\gamma\cdot\mathbf{n})\right].$$

This operator is Hermitian and has some simple properties, e. g.:

$$\hat{S}^{(p)}(k)\hat{S}^{(p)}(-k)=p,\ \hat{S}^{(-p)}(k)=ip\hat{S}^{(p)}(k)(\gamma\cdot\mathbf{n}).$$

Note also that the equation (38) can be re-written in the form similar to standard one:

$$\hat{\mathbf{K}}\Phi_{k,m}^{(p)}(E;\mathbf{r})=\sqrt{\frac{\kappa+p\lambda}{2\lambda}}\frac{\lambda+\varepsilon\kappa p}{2\lambda x}\begin{pmatrix}u_{+1}(\varepsilon;x)\chi_m^{kp} \\ iu_{-1}(\varepsilon;x)\chi_m^{-kp}\end{pmatrix},$$

where

$$\begin{pmatrix}u_{+1}(\varepsilon;x) \\ u_{-1}(\varepsilon;x)\end{pmatrix}=\begin{pmatrix}1 & s\frac{\alpha Z}{\kappa p+\lambda} \\ s\frac{\alpha Z}{\kappa p+\lambda} & 1\end{pmatrix}\begin{pmatrix}\phi_k(\varepsilon;x) \\ \frac{\sqrt{1-\varepsilon^2}}{\lambda+\varepsilon\kappa p}\hat{D}(k;x)\phi_k(\varepsilon;x)\end{pmatrix} \quad (40)$$

The action of $\hat{D}(k;x)$ on a regular and an irregular solution of (16) may be presented in the simplest form, if we choose the radial parts ϕ_k as follows ($\delta_s=(s+1)/2$):

$$\phi_k^{ir}(\varepsilon;x)\equiv\varphi_k^{ir}(\varepsilon;x)=W_{\eta,\lambda+s/2}(x),$$

$$\phi_k^r(\varepsilon;x)=\frac{\Gamma(\lambda-\eta+\delta_s)}{\Gamma(2\lambda+2\delta_s)}M_{\eta,\lambda+s/2}(x). \qquad (41)$$

These functions have the unit Wronskian, and so are more suitable, e. g., for the representing the Green function. In particular, $\phi_k^r(\varepsilon;x)$ has a simplest form for the continuum solution case (cf. with (18))

$$\frac{1}{x}\phi_k^r(\varepsilon;x)=\exp\left(-\frac{\pi}{2}\xi-i\Delta_k\right)F_k(\varepsilon;x).$$

The operators $\hat{D}(k;x)$ have a remarkable property to transform one type of radial functions into another

$$\hat{D}(k;x)\phi_k(\varepsilon;x)=a_k\phi_{-k}(\varepsilon;x), \qquad (42)$$

where $a_k^r=\lambda-s\eta$, $a_k^{ir}=-\lambda-s\eta$. Two useful properties for these coefficients play an important role:

$$a_k^r=-a_{-k}^{ir},\ a_k a_{-k}=\lambda^2-\eta^2=-a_k^r a_k^{ir}.$$

The identities (42) may be derived using the following recurrence relations between Whittaker functions with $s=\pm1$

$$\left(\frac{d}{dx}+s\frac{\lambda}{x}-s\frac{\eta}{2\lambda}\right)W_{\eta,\lambda+s/2}(x)=-\frac{\lambda+s\eta}{2\lambda}W_{\eta,\lambda-s/2}(x),$$

$$\left(\frac{d}{dx}+s\frac{\lambda}{x}-s\frac{\eta}{2\lambda}\right)M_{\eta,\lambda+s/2}(x)=$$

$$=(2\lambda+1)\left(\frac{\sqrt{\lambda^2-\eta^2}}{2\lambda(2\lambda+1)}\right)^{1-s}M_{\eta,\lambda-s/2}(x),$$

which are easy verified with the use of well-known recurrence relations for the confluent hypergeometric function (Gradshtein and Ryzhik 1967).

Two fundamental identities may be derived from the equations (38), (42)

$$\hat{\mathbf{K}}\Phi_{k,m}^{(p)}(E;\mathbf{r})=spa_k\frac{\sqrt{1-\varepsilon^2}}{\lambda-\varepsilon\kappa p}\hat{\mathbf{K}}\Phi_{-k,m}^{(-p)}(E;\mathbf{r}), \qquad (43)$$

$$\hat{\mathbf{K}}\Phi_{k,m}^{(p)}(E;\mathbf{r})=\frac{1}{2\lambda}\left[(\lambda+\varepsilon\kappa p)\Phi_{k,m}^{(p)}(E;\mathbf{r})+spa_k\sqrt{1-\varepsilon^2}\Phi_{-k,m}^{(-p)}(E;\mathbf{r})\right] \qquad (44)$$

These identities hold for each of four regular and irregular solutions $\Phi_{k,m}^{(p)}(E;\mathbf{r})$ of the second-order Dirac equation, and include all the information about the relations between the linear and second-order Dirac equation solutions. The expression (34) for fixed j contains two different solutions, with $k=\pm\kappa$. As is clear from the definition (15), $\Phi_{k,m}^{(p)}(E;\mathbf{r})$ has six pairs of functions with different eigenvalues of operator $\hat{K}$, $K=\pm\kappa$ and $p=\pm1$. In particular, $\Phi^{(1)}\equiv\Phi_{k'=\kappa,m}^{(p)}(E;\mathbf{r})$, and $\Phi^{(2)}\equiv\Phi_{k,m}^{(p=\pm1)}(E;\mathbf{r})$ may be treated as two of such pairs. The term «pair» for each of these functions means that, e. g., in the function $\Phi^{(1)}$ the index k' is fixed, $k'=\kappa$, and p takes two values, $p=\pm1$, *e.t.c.* The identity (43) shows that two other pairs, $\Phi^{(3)}\equiv\Phi_{k'=-\kappa,m}^{(p)}(E;\mathbf{r})$ and $\Phi^{(4)}\equiv\Phi_{k',m}^{(p=-1)}(E;\mathbf{r})$, generate the same solution of linear Dirac equation as the pairs $\Phi^{(1)}$ and $\Phi^{(2)}$, except for an inessential numerical factor. Thus, any of four functions $\Phi^{(i)}$ with i = 1,2,3,4 may be used to construct the solution of linear Dirac equation in terms of the solutions of squared equation (4). Obviously, that for all these cases the linear Dirac equation solution should have different functional forms. Note, that two additional pairs, $\Phi^{(5)}$ and $\Phi^{(6)}$, differed from $\Phi^{(i)}$ may be composed as the pairs with $p=s=+1$, $p=s=-1$, $p=-s=+1$, $p=-s=-1$. Nevertheless, these pairs don't generate a new functional form of the linear Dirac equation solution, because both functions in each of these pairs are eigenfunctions of the operator $\hat{K}$ with the same value $K=\kappa$ for $\Phi^{(5)}$ and $K=-\kappa$ for $\Phi^{(6)}$. Finally, the identity (44) demonstrates that although the squared operator $\hat{\mathbf{K}}$ acts only on one pair of the second-order Dirac equation solutions, the result involves all four solutions of (15) with fixed k. Namely, the solution of (1) with fixed s is a combination of two second-order Dirac equation solutions with different $k=\pm\kappa$. This fact is evident, because the squared operator doesn't commute with $\hat{K}$. Finally, the matrix structure of the right-hand side of the equation (44) explains the origin of the operator $\hat{S}^{(p)}(k)$ in the general matrix structure (39) of the linear Dirac equation solution (see also the operators $\hat{S}(k)$ and $\hat{S}'(k)$ in eqs. (45) and (47) bellow). Indeed, each of the bispinors $\Phi_{k,m}^{(\pm p)}(E;\mathbf{r})$ in (44) may be written in terms of operators $\hat{S}(\pm k)$ (8) acting on the eigenbispinors of β with opposite signs $p=\pm1$ and $k=\pm\kappa$. To present the sum of two terms in the right-hand side of eq. (44) in the compact operator form (39), one operator, $\hat{S}^{(p)}(k)$,

was introduced instead of a linear combination of two operators $\hat{S}(\pm k)$.

As was discussed above, the resulting expressions of linear Dirac equation solutions my be presented in different forms. First of them follows from (39) or (40) at $s=+1$ with the subsequent substitution $p\kappa\to k$ and $p\to s$ determining the quantum number k. The result in this case is

$$\Psi_{k,m}^{(1)}(E;\mathbf{r})=\hat{\mathbf{K}}\Phi_{\kappa,m}^{(p=s)}(E;\mathbf{r})=$$

$$=\frac{\lambda+\varepsilon k}{2\lambda x}\hat{S}(k)\begin{pmatrix}\phi_\kappa(\varepsilon;x)\chi_m^k(\mathbf{n})\\ ia_k\frac{\sqrt{1-\varepsilon^2}}{\lambda+\varepsilon k}\phi_{-\kappa}(\varepsilon;x)\chi_m^{-k}(\mathbf{n})\end{pmatrix}, \qquad (45)$$

where

$\hat{S}(k)=\sqrt{\frac{\kappa+s\lambda}{2\lambda}}\left[1+i\frac{\alpha Z}{k+\lambda}(\gamma\cdot\mathbf{n})\right]$. The presentation of this solution in the form similar to (40) (i. e, similar to the standard one) is

$$\Psi_{k,m}^{(1)}(E;\mathbf{r})=\sqrt{\frac{\kappa+s\lambda}{2\lambda}}\frac{\lambda+\varepsilon k}{2\lambda x}\begin{pmatrix}v_{+1}(\varepsilon;x)\chi_m^k\\ iv_{-1}(\varepsilon;x)\chi_m^{-k}\end{pmatrix}, \qquad (46)$$

where

$$\begin{pmatrix}v_{+1}(\varepsilon;x)\\ v_{-1}(\varepsilon;x)\end{pmatrix}=\begin{pmatrix}1 & \frac{\alpha Z}{k+\lambda}\\ \frac{\alpha Z}{k+\lambda} & 1\end{pmatrix}\begin{pmatrix}\phi_k(\varepsilon;x)\\ a_k\frac{\sqrt{1-\varepsilon^2}}{\lambda+\varepsilon k}\phi_{-k}(\varepsilon;x)\end{pmatrix}.$$

Another form of $\Psi_{k,m}(E;\mathbf{r})$ follows from (39), (40) at $p=1$. In this case the parameter k in (39), (40) is identical with the quantum number k of the linear Dirac equation, and one can find

$$\Psi_{k,m}^{(2)}(E;\mathbf{r})=\hat{\mathbf{K}}\Phi_{k,m}^{(p=\pm1)}(E;\mathbf{r})=$$

$$=\frac{\lambda+\varepsilon\kappa}{2\lambda x}\hat{S}'(k)\begin{pmatrix}\phi_\kappa(\varepsilon;x)\chi_m^k(\mathbf{n})\\ ia_k\frac{\sqrt{1-\varepsilon^2}}{\lambda+\varepsilon\kappa}\phi_{-\kappa}(\varepsilon;x)\chi_m^{-k}(\mathbf{n})\end{pmatrix}, \qquad (47)$$

where $\hat{S}'(k)=\sqrt{\frac{\kappa+\lambda}{2\lambda}}\left[1+i\frac{\alpha Z}{\kappa+\lambda}(\gamma\cdot\mathbf{n})\right]$. The presentation of this solution in the form similar to (34), (40) gives an equivalent formula

$$\Psi_{k,m}^{(2)}(E;\mathbf{r})=\sqrt{\frac{\kappa+\lambda}{2\lambda}}\frac{\lambda+\varepsilon\kappa}{2\lambda x}\begin{pmatrix}g_{+1}(\varepsilon;x)\chi_m^k\\ ig_{-1}(\varepsilon;x)\chi_m^{-k}\end{pmatrix}. \qquad (48)$$

where

$$\begin{pmatrix}g_{+1}(\varepsilon;x)\\ g_{-1}(\varepsilon;x)\end{pmatrix}=\begin{pmatrix}1 & s\frac{\alpha Z}{\kappa+\lambda}\\ s\frac{\alpha Z}{\kappa+\lambda} & 1\end{pmatrix}\begin{pmatrix}\phi_k(\varepsilon;x)\\ a_k\frac{\sqrt{1-\varepsilon^2}}{\lambda+\varepsilon\kappa}\phi_{-k}(\varepsilon;x)\end{pmatrix}.$$

The functions $\Phi^{(3)}$, $\Phi^{(4)}$ generate two additional expressions for $\Psi_{k,m}(E;\mathbf{r})$:

$$\Psi_{k,m}^{(3)}(E;\mathbf{r})=\hat{\mathbf{K}}\Phi_{-\kappa,m}^{(p=-s)}(E;\mathbf{r})=\frac{\lambda-\varepsilon k}{2\lambda x}\sqrt{\frac{\kappa-s\lambda}{2\lambda}}\times$$

$$\times\left[1+i\frac{\alpha Z}{\kappa-\lambda}(\gamma\cdot\mathbf{n})\right]\begin{pmatrix}\phi_{-\kappa}(\varepsilon;x)\chi_m^k(\mathbf{n})\\ ia_{-\kappa}\frac{\sqrt{1-\varepsilon^2}}{\lambda-\varepsilon k}\phi_{-\kappa}(\varepsilon;x)\chi_m^{-k}(\mathbf{n})\end{pmatrix}, \qquad (49)$$

$$\Psi_{k,m}^{(4)}(E;\mathbf{r})=\hat{\mathbf{K}}\Phi_{k,m}^{(p=-1)}(E;\mathbf{r})=\frac{\lambda-\varepsilon\kappa}{2\lambda x}\sqrt{\frac{\kappa-\lambda}{2\lambda}}\times$$

$$\times\left[1+i\frac{\alpha Z}{\kappa-\lambda}(\gamma\cdot\mathbf{n})\right]\begin{pmatrix}\phi_{-k}(\varepsilon;x)\chi_m^k(\mathbf{n})\\ ia_{-\kappa}\frac{\sqrt{1-\varepsilon^2}}{\lambda-\varepsilon\kappa}\phi_k(\varepsilon;x)\chi_m^{-k}(\mathbf{n})\end{pmatrix}, \qquad (50)$$

The radial functions $\phi(\varepsilon;x)$ and the coefficients a in all above expressions are determined by equations (41), (42) for both, regular and irregular solutions.

As is clear from eqs. (45) - (50), the form of radial parts in four solutions $\Psi_{k,m}^{(i)}(E;\mathbf{r})$ differs from the standard one, because these solutions involve the Whittaker functions with quite different parameters comparing with the standard solution (36). One can use the relations between adjacent Whittaker functions to find a connection of radial parts in eqs. (45) - (50) with functions $f_p(E;r)$ in (36). As an example, for the regular and irregular solution such relations are

$$\sqrt{x}M_{\eta,\lambda+\frac{1}{2}}(x)=(2\lambda+1)\left[M_{\eta,\lambda-\frac{1}{2}}(x)-M_{\eta,\lambda+\frac{1}{2}}(x)\right],$$

$$2\lambda\sqrt{x}M_{\eta,\lambda-\frac{1}{2}}(x)=(\lambda-\eta)M_{\eta,\lambda-\frac{1}{2}}(x)+(\lambda+\eta)M_{\eta,\lambda+\frac{1}{2}}(x),$$

$$\sqrt{x}W_{\eta,\lambda\pm\frac{1}{2}}(x)=W_{\eta,\lambda+\frac{1}{2}}(x)+(\eta\mp\lambda)W_{\eta,\lambda-\frac{1}{2}}(x).$$

The direct calculation demonstrates the coincidence of all the above-discussed solutions $\Psi^{(i)}_{k,m}(E;\mathbf{r})$ with the standard solution $\Psi_{k,m}(E;\mathbf{r})$ in equation (36) and gives the appropriate r-independent proportionality coefficients. More precisely, for the solution $\Psi^{(1)}_{k,m}(E;\mathbf{r})$ in form (46) the coefficients C_k in the following expression

$$\Psi_{k,m}(E;\mathbf{r})=\frac{C_k}{r}\begin{pmatrix} v_{+1}(\varepsilon;x)\chi^k_m(\mathbf{n}) \\ iv_{-1}(\varepsilon;x)\chi^{-k}_m(\mathbf{n})\end{pmatrix}$$

for regular and irregular solutions are

$$C^r_k=\frac{\Gamma(2\lambda)}{\Gamma(\lambda-\eta)}\sqrt{1+\varepsilon}(k+\lambda+\eta-Z\nu),$$

$$C^{ir}_k=\frac{1}{2\lambda}\sqrt{1+\varepsilon}(k+\lambda-\eta+Z\nu).$$

Here Γ-functions appear according to our definition of the regular solution in the form (41). These coefficients can be also derived by the comparison of an asymptotic behaviour for the appropriate solutions at $r\to 0$ or $r\to\infty$.

Despite different forms, the radial functions in all $\Psi^{(i)}_{km}$ involve the same Whittaker functions. For an example, the functions $g_{\pm1}$ and $v_{\pm1}$ in equations (46), (48) are identical at $k=\kappa$. At $k=-\kappa$ they differ from each other by the r-independent coefficient:

$$v_{\pm1}(\varepsilon;x)=\left[a_k\frac{\alpha Z\sqrt{1-\varepsilon^2}}{(\kappa-\lambda)(\varepsilon\kappa-\lambda)}\right]^{(1-s)/2}g_{\pm1}(\varepsilon;x).$$

In the case of $\alpha Z=0$, functions $g^r_{\pm1}$ and $g^{ir}_{\pm1}$ involve only one Whittaker function, which is a regular and an irregular solution of radial Schrödinger equation for the Coulomb problem. Different forms, (45) - (50), of linear Dirac equation solutions may be useful in the concrete relativistic calculations.

Obviously, the above-mentioned fundamental systems of solutions for the linear Dirac equation at arbitrary energy E are sufficient for deriving of all the information on the problem, i. e., eigenfunctions of bound and continuum states, Green function, *e.t.c.* Nevertheless, in the next Section we shall derive the Dirac-Coulomb Green function by a simpler method, namely, as a result of the direct action of the squared operator on the Green function of the second-order Dirac equation.

4. Green function of the linear Dirac equation

We define the Dirac-Coulomb Green function as the solution of the following equation (see (25))

$$[\hat{H}(r)-E]G_E(\mathbf{r},\mathbf{r}')=\beta\delta(\mathbf{r}-\mathbf{r}').$$

The solution of this equation in terms of standard Dirac equation solutions (36) is well-known, and was derived first by Wichmann and Kroll (1956). The result can be presented in the following form (with the preceeding notations):

$$G_E(\mathbf{r},\mathbf{r}')=-\frac{2m_e}{\hbar^2a_0\nu}\sum_{k,m}\frac{\Gamma(\lambda-\eta)}{\Gamma(2\lambda+1)}\Psi^r_{k,m}(E;\mathbf{r})\overline{\Psi^{ir}_{k,m}(E;\mathbf{r}')},$$

$$r<r'. \tag{51}$$

In the case $r>r'$ one has to replace $\Psi^r_{k,m}(E;\mathbf{r})\overline{\Psi^{ir}_{k,m}(E;\mathbf{r}')}\to\Psi^{ir}_{k,m}(E;\mathbf{r})\overline{\Psi^r_{k,m}(E;\mathbf{r}')}$. It is important to note that in all formulas for the Green function of this Section, the sign of Dirac-conjugation is related only to a matrix structure of corresponding functions and do not suppose a complex conjugation of their radial parts (which are complex outside the interval $-m_ec^2<E<m_ec^2$), i. e., we assume the following convention: $\overline{f(r)\theta}=f(r)\overline{\theta}$. Actually, the result (51) is the partial wave expansion of $G_E(\mathbf{r},\mathbf{r}')$, which may be written also in the matrix form:

$$G_E(\mathbf{r},\mathbf{r}')=\sum_{k,m}G^{(E)}_{k,m}(\mathbf{r},\mathbf{r}')=$$

$$=\sum_{k,m}\begin{pmatrix} G^{11}_{k,m}(r,r')\chi^k_m\chi^{k\dagger}_m & iG^{12}_{k,m}(r,r')\chi^k_m\chi^{-k\dagger}_m \\ iG^{21}_{k,m}(r,r')\chi^{-k}_m\chi^{k\dagger}_m & -G^{22}_{k,m}(r,r')\chi^{-k}_m\chi^{-k\dagger}_m\end{pmatrix}. \tag{52}$$

The significant difficulty of using the expression (52) occur, when it is necessary to integrate $G_E(\mathbf{r},\mathbf{r}')$ over radial variables calculating the matrix elements, because this presentation of G_E has no symmetric form in variables r and r'. Some symmetric expressions for radial parts of $G^{(E)}_{k,m}$ in (52) were discussed by Zon *et al* (1972) (see also Borovskii *et al* (1995)).

We derive below a number of representations for $G_E(\mathbf{r},\mathbf{r}')$ on the basis of the second-order Dirac

equation approach, i. e., in the accordance with (26), by the direct action of the squared operator $\hat{\mathbf{K}}$ on the Green function $\mathcal{G}_E(E;\mathbf{r},\mathbf{r}')$ in forms (27) - (32) or (33). We note here that, using the functions $\phi^r_k(\varepsilon;x)$ and $\phi^{ir}_k(\varepsilon;x)$ introduced in (41), the function $\mathcal{G}_E(E)$ may be presented in the form equivalent to (27, 28)

$$\mathcal{G}_E(E;\mathbf{r},\mathbf{r}')=\frac{4m_e}{\hbar^2a_0\nu}\sum_{kmp}p\Phi^{(p)r}_{k,m}(E;\mathbf{r})\overline{\Phi^{(p)ir}_{k,m}(E;\mathbf{r})},$$

$$r<r'. \tag{53}$$

We derive first $G_E(\mathbf{r},\mathbf{r}')$ from the Sturmian expansion of $\mathcal{G}_E(E;\mathbf{r},\mathbf{r}')$. Similarly to (37), (38) the action of $\hat{\mathbf{K}}$ on the Sturmian function (23) may be presented as follows

$$\hat{\mathbf{K}}S^{(p)}_{nkm}=\frac{1}{2\lambda x}\left[(\lambda+\varepsilon\kappa p)\phi_{nk}(x)-i\,sp\hat{D}(k;x)\phi_{nk}(x)(\alpha\cdot\mathbf{n})\right]\times$$

$$\times\theta^{(p)}_{km}(\mathbf{n}).$$

Here the simple identity, $(\alpha\cdot\mathbf{n})\theta^{(p)}_{km}(\mathbf{n})=-i\,sp\theta^{(-p)}_{-km}(\mathbf{n})$, was used. The action of $\hat{D}(k;x)$ on the radial part of the Sturmian function $\phi_{nk}(x)$ (see (24)), similarly to (42), is

$$\hat{D}(k;x)\phi_{nk}(x)=s(\overline{\eta}_n-\eta)\phi_{nk}(x)+s\sqrt{\overline{\eta}_n^2-\lambda^2}\,\phi_{n+s,-k}(x),$$

where $\overline{\eta}_n=n+\lambda+\delta_s$. As a result, the action of $\hat{\mathbf{K}}$ on the Green function of the second-order Dirac equation in the form (32) or (33) may be presented as follows

$$G_E(\mathbf{r},\mathbf{r}')=\sum_{k,m}G^{(E)}_{k,m}(\mathbf{r},\mathbf{r}'), \tag{54}$$

$$G_E(\mathbf{r},\mathbf{r}')=\sum_p\frac{1}{2\lambda}\left[(\lambda+\varepsilon\kappa p)g_k(E;r,r')+i\,sg^{(1)}_k(E;r,r')(\alpha\cdot\mathbf{n})\right]\times$$

$$\times p\theta^{(p)}_{k,m}(\mathbf{n})\overline{\theta^{(p)}_{k,m}(\mathbf{n}')},$$

where $g_k(E;r,r')$ is given by (32), and where the function $g^{(1)}_k(E;r,r')$ is

$$g^{(1)}_k(E;r,r')=\frac{4m_ec^2(1-\varepsilon^2)}{\hbar^3\sqrt{xx'}}\left[\delta(x-x')+(xx')^{\lambda}\left(\frac{x}{x'}\right)^{s/2}\times\right.$$

$$\left.\times e^{-(x+x')/2}\sum_{n=(1-s)/2}^{\infty}\frac{(n+\delta_s)!L^{2\lambda-s}_n(x)L^{2\lambda+s}_n(x')}{\Gamma(n+2\lambda+\delta_s)(\overline{\eta}_n-\eta)}\right]. \tag{55}$$

The sum over $p=\pm1$ in (54) may be calculated explicitly. For this purpose it is convenient to use the functions $\Theta^{(p)}_{km}$ instead of $\theta^{(p)}_{km}$ in (54). It is possible to do that, because the phase factors $e^{\pm i\pi s(p-1)/4}$ (see (14)) cancel in the product of two angular functions. Thus, the following identity is valid for $\xi=0$ and 1:

$$\sum_p p^{\xi}\theta^{(p)}_{k,m}(\mathbf{n})\overline{\theta^{(p)}_{k,m}(\mathbf{n}')}=$$

$$=\hat{S}(k;\mathbf{n})\begin{pmatrix}\chi^k_m(\mathbf{n})\chi^{k\dagger}_m(\mathbf{n}') & 0 \\ 0 & (-1)^{\xi+1}\chi^k_m(\mathbf{n})\chi^{k\dagger}_m(\mathbf{n}')\end{pmatrix}\hat{S}(k;\mathbf{n}').$$

Thus, $G_E(\mathbf{r},\mathbf{r}')$ may be presented in a matrix form involving the operator $\hat{S}(k;\mathbf{n})$ (8). Nevertheless, we consider the expression for $G_E(\mathbf{r},\mathbf{r}')$ in the form (54) as convenient for applications too, because it has the form of a direct product of two bispinors. Such form is very useful especially to separate radial and spin-angular variables in matrix elements of the interelectron interaction in the many-body perturbation theory on the basis of Coulomb solutions.

The action of operator $\hat{\mathbf{K}}$ on the Green function (53) (or, equivalent, on the (27), (28)) generates other representations for $G_E(\mathbf{r},\mathbf{r}')$, in terms of regular and irregular solutions (45) - (50). We shall demonstrate some details of calculations for the case, when only functions (45) are used. Considering this case, before the action of operator $\hat{\mathbf{K}}$, it is convenient to separate explicitly the sum over k in the expression (53) into two terms, with $k=\kappa$ and $k=-\kappa$. After them, substituting $p\to-p$ in the term with $k=-\kappa$, we obtain:

$$I=\hat{\mathbf{K}}\sum_{kmp}p\Phi^{(p)r}_{k,m}(E;\mathbf{r})\overline{\Phi^{(p)ir}_{k,m}(E;\mathbf{r}')}=\sum_{\kappa mp}p\hat{\mathbf{K}}\Phi^{(p)r}_{\kappa,m}(E;\mathbf{r})\times$$

$$\times\overline{\Phi^{(p)ir}_{\kappa,m}(E;\mathbf{r}')}-\sum_{\kappa mp}p\hat{\mathbf{K}}\Phi^{(-p)r}_{-\kappa,m}(E;\mathbf{r})\overline{\Phi^{(-p)ir}_{-\kappa,m}(E;\mathbf{r}')}$$

Using the identity (43), it is possible to clculate the action of operator $\hat{\mathbf{K}}$ in the second term on the right hand side of above relation. Then the expression for I is reduced as follows:

$$I=\sum_{\kappa mp}p\hat{\mathbf{K}}\Phi^{(p)r}_{\kappa,m}(E;\mathbf{r})\left[\overline{\Phi^{(p)ir}_{\kappa,m}(E;\mathbf{r}')}-\right.$$

$$\left.-pa^r_{-\kappa}\frac{\sqrt{1-\varepsilon^2}}{\lambda+\varepsilon\kappa p}\overline{\Phi^{(-p)ir}_{\kappa,m}(E;\mathbf{r}')}\right].$$

The above-mentioned relation $a^{r}_{-\kappa}=-a^{ir}_{-\kappa}$ and the identity (44) lead finally to the fact that the expression in the square brackets is the irregular solution $\mathbf{K}\Phi^{(p)\,ir}_{\kappa,m}$ of the Dirac equation. Therefore, the following result is obtained for the Green function

$$G_E(\mathbf{r},\mathbf{r}')=\frac{4m_e}{\hbar^2 a_0\nu}\sum_{\kappa m p}\frac{2\lambda p}{\lambda+\varepsilon\kappa p}\hat{\mathbf{K}}\Phi^{(p)\,r}_{\kappa,m}(E;\mathbf{r})\overline{\hat{\mathbf{K}}\Phi^{(p)\,ir}_{\kappa,m}(E;\mathbf{r}')},$$

or, in the accordance with (45),

$$G_E(\mathbf{r},\mathbf{r}')=\frac{4m_e}{\hbar^2 a_0\nu}\sum_{km}\frac{2\lambda s}{\varepsilon k+\lambda}\Psi^{(1)r}_{km}(E;\mathbf{r})\overline{\Psi^{(1)ir}_{km}(E;\mathbf{r}')}.\quad(56)$$

It is clear that above manipulations do not depend on a relation between r and r'. In a similar way, it is easy to derive the expressions for $G_E(\mathbf{r},\mathbf{r}')$ in terms of other functions $\Psi^{(i)}_{km}(E;\mathbf{r})$ discussed in Sec. 3:

$$G_E(\mathbf{r},\mathbf{r}')=\frac{4m_e}{\hbar^2 a_0\nu}\sum_{km}\frac{2\lambda}{\varepsilon\kappa+\lambda}\Psi^{(2)r}_{km}(E;\mathbf{r})\overline{\Psi^{(2)ir}_{km}(E;\mathbf{r}')}=\quad(57)$$

$$=\frac{4m_e}{\hbar^2 a_0\nu}\sum_{km}\frac{2\lambda s}{\varepsilon k-\lambda}\Psi^{(3)r}_{km}(E;\mathbf{r})\overline{\Psi^{(3)ir}_{km}(E;\mathbf{r}')}=\quad(58)$$

$$=\frac{4m_e}{\hbar^2 a_0\nu}\sum_{km}\frac{2\lambda s}{\varepsilon\kappa-\lambda}\Psi^{(4)r}_{km}(E;\mathbf{r})\overline{\Psi^{(4)ir}_{km}(E;\mathbf{r}')}.\quad(59)$$

Obviously, the expressions (56) -(59) are similar to (51), and they may by derived also as a direct product of appropriated fundamental solutions divided by their Wronskian. In our approach the calculations of these Wronskians were not necessary. For the brevity, we shall analuse below only the result for $G_E(\mathbf{r},\mathbf{r}')$ in the form (56). The corresponding results for other forms may be obtained by a similar way.

Using eq. (45) for $\Psi^{(1)r}_{km}(E;\mathbf{r})$ and simple auxiliary identities:

$$(1-\varepsilon^2)(\lambda^2-\eta^2)=\lambda^2-k^2\varepsilon^2,\quad \hat{S}(k)\beta=s\beta\hat{S}^{-1}(k),$$

$$\hat{S}(k)=\sqrt{\frac{\kappa+s\lambda}{2\lambda}}\left[1+i\frac{\alpha Z}{k+\lambda}(\gamma\cdot\mathbf{n})\right],$$

we obtain (cf. with (52)):

$$G_E(\mathbf{r},\mathbf{r}')=\sum_{k,m}G^{(E)}_{k,m}(\mathbf{r},\mathbf{r}')=$$

$$=\sum_{km}\hat{S}(k)\begin{pmatrix} g_k^{(11)}\chi^k_m\chi^{k\dagger}_m & ig_k^{(12)}\chi^k_m\chi^{-k\dagger}_m \\ ig_k^{(21)}\chi^{-k}_m\chi^{k\dagger}_m & -g_k^{(22)}\chi^{-k}_m\chi^{-k\dagger}_m\end{pmatrix}\hat{S}^{-1}(k).\quad(60)$$

Here the diagonal radial parts, $g_k^{(ii)}(E;r,r')$, are the same as radial parts of $\mathcal{G}_E(E;\mathbf{r},\mathbf{r}')$. The off-diagonal radial parts of the Green function, $g_k^{(12)}(E;r,r')$ and $g_k^{(21)}(E;r,r')$, can be received by the action of the operator $\hat{D}$ on the radial parts of $\mathcal{G}_E(E;\mathbf{r},\mathbf{r}')$. As the result, we have:

$$g_k^{(11)}=\frac{4m_e}{\hbar^2 a_0\nu}\frac{k\varepsilon+\lambda}{2\lambda xx'}\phi^r_k(\varepsilon;x_<)\phi^{ir}_k(\varepsilon;x_>)=\frac{k\varepsilon+\lambda}{2\lambda}g_k(E;r,r')$$

$$g_k^{(22)}=\frac{4m_e}{\hbar^2 a_0\nu}\frac{1-\varepsilon^2}{2\lambda(k\varepsilon+\lambda)xx'}D(\kappa;x)D(\kappa;x')\times$$

$$\times\phi^r_k(\varepsilon;x_<)\phi^{ir}_k(\varepsilon;x_>)=\frac{k\varepsilon-\lambda}{2\lambda}g_{-k}(E;r,r')$$

$$g_k^{(12)}=\frac{4m_e}{\hbar^2 a_0\nu}\frac{\sqrt{1-\varepsilon^2}}{2\lambda xx'}D(\kappa;x')\phi^r_k(\varepsilon;x_<)\phi^{ir}_k(\varepsilon;x_>)=$$

$$=\frac{\sqrt{1-\varepsilon^2}}{2\lambda}D(\kappa;x')g_k(E;r,r')\quad(61)$$

$$g_k^{(21)}=\frac{\sqrt{1-\varepsilon^2}}{2\lambda}D(\kappa;x)g_k(E;r,r')=$$

$$=-\frac{\sqrt{1-\varepsilon^2}}{2\lambda}D(-\kappa;x')g_{-k}(E;r,r')\quad(62)$$

Equations (61) and (62) demonstrate explicitly the symmetry relation:

$$g_k^{(12)}(E;r,r')=g_k^{(21)}(E;r',r),$$

which is evident also from a more general identity for $G_E(\mathbf{r},\mathbf{r}')$:

$$G_E^{\dagger}(\mathbf{r},\mathbf{r}')=\beta G_E^{*}(\mathbf{r}',\mathbf{r})\beta.$$

The above expressions present the simplest representation of Dirac-Coulomb Green function in terms of the radial part of $\mathcal{G}_E(\mathcal{E};\mathbf{r},\mathbf{r}')$. Each of the expressions (28) - (32) for $g_k(E;r,r')$ may be used here in concrete applications. In particular,

the action of $D(\kappa;x)$ on $g_k(E;r,r')$ in the form (32) gives the result similar to (55):

$$g_k^{(21)}=\frac{2m_e^2c(1-\varepsilon^2)}{\hbar^3\lambda}[S_1(x,x')+S_2(x,x')],\quad(63)$$

where S_1 and S_2 are series of Laguerre polynomials:

$$S_1=\exp\left(-\frac{x+x'}{2}\right)(xx')^{\lambda-1/2}\sqrt{\frac{x'}{x}}\sum_{n=0}^{\infty}\frac{(n+1)!L^{2\lambda+1}_{n+1}(x)L^{2\lambda+1}_n(x')}{(n+\lambda+1-\eta)\Gamma(2\lambda+n+1)}\quad(64)$$

$$S_2=\exp\left(-\frac{x+x'}{2}\right)(xx')^{\lambda}\sum_{n=0}^{\infty}\frac{n!L^{2\lambda+1}_n(x)L^{2\lambda+1}_n(x')}{\Gamma(2\lambda+2+n)}=\frac{1}{\sqrt{xx'}}\delta(x-x')\quad(65)$$

The availability of the delta-like term (65) in (63) (see also (55)) is a purely formal circumstance. Indeed, as it follows from the general arguments, the terms on the principal diagonal of the Green function (52) should be continuos at $r=r'$, and only the off-diagonal terms contain the finite discontinuity. Thus, the sum (64) should be divergent at $r=r'$ to compensate the singularity of the term (65). This fact verifies easy with the use of asymptotic expansions for Laguerre polynomials at high n. To demonstrate this cancellation more precisely, we used the recurrence relations for Laguerre polynomials to obtain the following relation:

$$S_1+S_2=2\lambda x'S_3-(\eta+\lambda)S_4,$$

where S_3 and S_4 are

$$S_3=\exp\left(-\frac{x+x'}{2}\right)(xx')^{\lambda-1}\sum_{n=0}^{\infty}\frac{n!L^{2\lambda}_n(x)L^{2\lambda+1}_n(x')}{(2\lambda+1+n)\Gamma(n+\lambda+1-\eta)},$$

$$S_4=\exp\left(-\frac{x+x'}{2}\right)(xx')^{\lambda}\sum_{n=0}^{\infty}\frac{n!L^{2\lambda+1}_n(x)L^{2\lambda+1}_n(x')}{(2\lambda+2+n)\Gamma(n+\lambda+1-\eta)}.$$

The simple analysis of the asymptotic expansions of $L^{\alpha}_{\eta}(x)$ shows, that S_3 and S_4 are finite ones at $r=r'$. Therefore, the sum S_1+S_2 doesn't contains a singularity in the accordance with a general theory of Green functions. Thus, the remark of Swainson and Drake (1991) on the absence of δ-functions in the off-diagonal terms of the Dirac-Coulomb Green function obtained by Zapriagaev and Manakov (1976) is wrong.

All symmetric in terms of radial variables expressions for the Dirac-Coulomb Green function were tested by the direct analytical calculation of the left hand side of the following identity

$$\langle nk|G(E)|nk\rangle=1/(E_{nk}-E).$$

5. Bound and continuum wavefunctions of the Dirac-Coulomb problem

To derive the Coulomb wavefunctions of bound and continuum states we shall use the Green functions. One of goals of these calculations is to demonstrate the validity of results obtained for the Green function. Besides, in such method the normalization of wavefunctions is determined automatically.

(i) *Bound-state wavefunctions*

The Green function $G_E(\mathbf{r},\mathbf{r}')$ as a function of a complex energy E has poles at the energies of bound states $E=E_{nk}$, where E_{nk} is determined by the equation (22). As is well-known, the normalized wavefunctions of bound states, $\Psi_{nkm}(\mathbf{r})$, may be derived as the residues of $G_E(\mathbf{r},\mathbf{r}')$ at $E=E_{nk}$ according to the relation

$$\mathrm{Res}\,G_E(\mathbf{r},\mathbf{r}')\Big|_{E=E_{nk}}=\sum_{k=\pm\kappa,m}\Psi_{nkm}(\mathbf{r})\overline{\Psi_{nkm}(\mathbf{r}')}.\quad(66)$$

Because the pole terms in partial-wave expansions (56) - (59) for G_E are Gamma-functions $\Gamma(\lambda+\delta_s-\eta)$ entered the reqular solution $\Psi^{(i)r}_{km}(E;\mathbf{r})$, the residues (66) are calculated easily using the identity

$$\mathrm{Res}\,\Gamma\left(\lambda+\delta_s-\frac{\alpha ZE}{\sqrt{(m_ec^2)^2-E^2}}\right)\Bigg|_{E=E_{nk}}=m_ec^2\frac{(-1)^{n_r-\delta_s}(\alpha Z)^2}{(n_r-\delta_s)!N^3}.$$

The explicit form of the corresponding bound-state wavefunction may be derived now for each of Green functions (56) - (59) taking into account the definition of $\Psi^{(i)r,ir}_{km}(E;\mathbf{r})$ and the identities (20).

We present below two forms of wavefunctions derived as residues of G_E in the forms (56) and (57). In the first case the wavefunction has the form similar to (45), (46):

$$\Psi^{(1)}_{nkm}(\mathbf{r})=C_{nk}\hat{S}(k;\mathbf{n})\begin{pmatrix} v_1(r)\chi^{k}_{m}(\mathbf{n}) \\ iv_2(r)\chi^{-k}_{m}(\mathbf{n})\end{pmatrix}, \qquad (67)$$

where the operator $\hat{S}(k;\mathbf{n})$ was defined in equation (45), and the coefficient C_{nk} is

$$C_{nk}=-s\left(\frac{2Z}{Na_0}\right)^{3/2}\sqrt{\frac{\varepsilon\kappa+s\lambda}{4\lambda N}\frac{(n_r-1)!}{\Gamma(n_r+2\lambda+1)}}.$$

The «large», v_1, and «small», v_2, components of the wavefunction in (67) are

$$v_1(r)=y^{\lambda}\exp\left(-\frac{y}{2}\right)L^{2\lambda+1}_{n_r-1}(y),$$

$$v_2(r)=s\frac{\alpha Z}{N}\frac{n_r(n_r+2\lambda)}{\varepsilon\kappa+s\lambda}y^{\lambda-1}\exp\left(-\frac{y}{2}\right)L^{2\lambda-1}_{n_r}(y),$$

$$y=\frac{2Zr}{Na_0}.$$

Another form of wavefunctions follows from the expression (57) for the Green function. In this case the calculation of the residue (66) gives

$$\Psi^{(2)}_{nkm}(\mathbf{r})=-\hat{S}'(k;\mathbf{n})\begin{pmatrix} g_1(r)\chi^{k}_{m}(\mathbf{n}) \\ ig_2(r)\chi^{-k}_{m}(\mathbf{n})\end{pmatrix}. \qquad (68)$$

Here $\hat{S}'(k;\mathbf{n})$ was introduced in (47), and radial parts g_1 and g_2 are:

$$g_1(r)=s\left(\frac{2Z}{Na_0}\right)^{3/2}\sqrt{\frac{\varepsilon\kappa+\lambda}{4N\lambda}\frac{\bar{n}_r!}{\Gamma(2\lambda+2\delta+\bar{n}_r)}}\,y^{\lambda+\delta-1}\times$$

$$\times\exp\left(-\frac{y}{2}\right)L^{2\lambda+s}_{\bar{n}_r}(y),$$

$$g_2(r)=\left(\frac{2Z}{Na_0}\right)^{3/2}\sqrt{\frac{\varepsilon\kappa-\lambda}{4N\lambda}\frac{(\bar{n}_r+s)!}{\Gamma(2\lambda+1+\bar{n}_r)}}\,y^{\lambda+\delta}\times$$

$$\times\exp\left(-\frac{y}{2}\right)L^{2\lambda-s}_{\bar{n}_r+s}(y).$$

Here $\delta=(1+s)/2$, $\bar{n}_r=n_r-\delta$. These functions were obtained previously by Zapriagaev (1987).

In the nonrelativistic limit, $\alpha Z\to 0$, we have $\hat{S}'(k;\mathbf{n})\to 1$, $g_2(r)\to 0$, $g_1(r)=sR_{nl}(r)$, where $R_{nl}(r)$ is the normalized nonrelativistic Coulomb wavefunction, $l=\kappa+(s-1)/2$.

The above expressions are simplified for the states with $n_r=0$. For these states $s=-1$ and one component of bispinors in (67), (68) is zero. Such bispinors are eigenfunctions of matrix β. As a result both forms lead to the same expression for $\Psi_{n=\kappa,k=-\kappa,m}(\mathbf{r})\equiv\Psi_{n_r=0}(\mathbf{r})$ involving the matrix instead of γ

$$\Psi_{n_r=0}(\mathbf{r})=\hat{\mathcal{S}}(-\kappa;\mathbf{n})\begin{pmatrix} f(r)\chi^{-\kappa}_{m}(\mathbf{n}) \\ 0\end{pmatrix}=f(r)\,\theta^{(+1)}_{-\kappa m}(\mathbf{n})=$$

$$=\frac{f(r)}{\sqrt{2\lambda}}\begin{pmatrix} \sqrt{\kappa+\lambda}\,\chi^{-\kappa}_{m}(\mathbf{n}) \\ -i\sqrt{\kappa-\lambda}\,\chi^{\kappa}_{m}(\mathbf{n})\end{pmatrix},$$

$$f(r)=\left(\frac{2Z}{na_0}\right)^{3/2}\frac{1}{\sqrt{2n\Gamma(2\lambda)}}\left(\frac{2Zr}{na_0}\right)^{\lambda-1}\exp\left(-\frac{Zr}{na_0}\right).$$

Here $\mathcal{S}(k;\mathbf{n})$ is the operator introduced in (8) for the squared Dirac equation solutions, and this function is simultaneously the solution of the second-order Dirac equation (see (15)). Note, that the case $n_r=0$ is the unique case, when the solution of the linear Dirac equation coincides with one of the squared equation solutions and therefore its spin-angular structure is determined by the operator $\mathcal{S}(k;\mathbf{n})$ in eq. (8).

(ii) *Wavefunctions of continuum states*

The normalized wavefunction of a continuum state, $\Psi_{Ekm}(\mathbf{r})$, may be derived on the basis of following arguments. The part of the spectral expansion $G^{(+)}_{E}(\mathbf{r},\mathbf{r}')$ for real $E>m_ec^2$ involving the integration over the positive continuum is (see Berestetskii, *et al* (1982))

$$G^{(+)}_{E}(\mathbf{r},\mathbf{r}')\sim\sum_{km}\int_{m_ec^2}^{\infty}\frac{dE'\,\Psi_{E'km}(\mathbf{r})\overline{\Psi_{E'km}(\mathbf{r}')}}{E'-E-i0}=$$

$$=\sum_{km}\mathcal{P}\int_{m_ec^2}^{\infty}\frac{dE'\,\Psi_{E'km}(\mathbf{r})\overline{\Psi_{E'km}(\mathbf{r}')}}{E'-E}+i\pi\sum_{km}\int_{m_ec^2}^{\infty}\Psi_{Ekm}(\mathbf{r})\overline{\Psi_{Ekm}(\mathbf{r}')} \qquad (69)$$

Here $\mathcal{P}$ denotes the principal part of an integral. An infinitesimal addition $-i\,0$ in the denominator of (69) (and the similar addition, $+i$, 0, in the integral over the negative continuum) fix the analytical structure of G_E in the plane of a complex energy E. Namely, G_E is the analytical function

Here $G^{(E=E_{n\kappa})}_{k',m'}(\mathbf{r},\mathbf{r}')$ with $k'\neq k$ is the same as in (60) or (54) if we put $E=E_{n\kappa}$ in these equations. So, the explicit form of this term is evident and we do not discuss it below.

Further, $\tilde{G}^{(E_{n\kappa})}_{km}(\mathbf{r},\mathbf{r}')$ is the «regular part» of $G^{(E)}_{km}$, i. e., there is $G^{(E)}_{km}$ at $E=E_{n\kappa}$ with extracted singular term. Finally, according to (72), (73) the terms $\mathcal{F}^{E_{n\kappa}}_{k,m}$ in (75) should be derived by the differentiation in ν of «pole parts». For example, these parts are the same for diagonal terms in (54) and (60), and they are equal to the quantities (74) multiplied by the factor

$$\frac{\gamma}{2\lambda}\frac{(\varepsilon k\pm\lambda)[(N/Z\nu)^2-1]}{\sqrt{1-(\alpha/\nu)^2}+\gamma/N}.$$

Note that in differentiating in ν of x, x' - dependent functions which are in fact the radial Sturmian functions (24) the following simple identity is useful

$$\left(y=\frac{2Zr}{Na_0},\, y'=\frac{2Zr'}{Na_0}\right)$$

$$\frac{d}{d\nu}[f(x(\nu))\phi(x'(\nu))]\Big|_{\nu=N/Z}=$$

$$=-\frac{Z}{N}\left[y\frac{df(y)}{dy}\phi(y')+y'f(y)\frac{d\phi(y')}{dy'}\right].$$

We present below separately the final expressions for the partial-wave terms

$$G^{(E_{n\kappa})}_{km}(\mathbf{r},\mathbf{r}')\equiv\tilde{G}^{(E_{n\kappa})}_{k,m}(\mathbf{r},\mathbf{r}')+\mathcal{F}^{E_{n\kappa}}_{k,m}(\mathbf{r},\mathbf{r}')$$

of the reduced Green function $G^{E_{n\kappa}}_{km}(\mathbf{r},\mathbf{r}')$ in the forms (54) and (60).

(i) The direct - products form of $G^{(E_{n\kappa})}_{km}(\mathbf{r},\mathbf{r}')$

According to equation (54) the function $G^{(E_{n\kappa})}_{km}(\mathbf{r},\mathbf{r}')$ has the following spin-angular structure

$$G^{(E_{n\kappa})}_{km}(\mathbf{r},\mathbf{r}')=\frac{m_e}{\hbar^2a_0}\frac{2Z}{\lambda N^2}\times$$

$$\times\sum_{p}\Big\{(k'\gamma+\lambda N)[\tilde{g}_k(y,y')+f^{(k')}_k(y,y')]+$$

$$+is(\alpha Z)[\tilde{g}^{(1)}_k(y,y')+f_k(y,y')](\boldsymbol{\alpha}\cdot\mathbf{n})\Big\}p\,\theta^{(p)}_{k,m}(\mathbf{n})\overline{\theta^{(p)}_{k,m}(\mathbf{n}')} \qquad (76)$$

We introduce here a special index, $k'\equiv p\kappa$, instead of p, which is useful for the below presented considerations. So, $k'=\pm\kappa$ for $p=\pm 1$.

The functions $\tilde{g}_k$ and $\tilde{g}^{(1)}_k$ are the «regular parts» of functions g_k and $g^{(1)}_k$ introduced in (54)

$$\tilde{g}_k(y,y')=(yy')^{\lambda+\delta_s-1}\exp\left(-\frac{y+y'}{2}\right)\times$$

$$\times\sum_{n=0}^{\infty}{}'\frac{n!\,L^{2\lambda+s}_{n}(y)L^{2\lambda+s}_{n}(y')}{\Gamma(n+2\lambda+2\delta_s)(n-n_r+\delta_s)}, \qquad (77)$$

$$\tilde{g}^{(1)}_k(y,y')=\frac{\delta(y-y')}{\sqrt{yy'}}+y^{\lambda-\delta_s}y'^{\lambda+\delta_s-1}\exp\left(-\frac{y+y'}{2}\right)\times$$

$$\times\sum_{n=(1-s)/2}^{\infty}{}'\frac{(n+\delta_s)!\,L^{2\lambda-s}_{n+s}(y)L^{2\lambda+s}_{n+s}(y')}{\Gamma(n+2\lambda+\delta_s)(n-n_r+\delta_s)}.$$

Here the prime in the sums over n denotes that $n\neq n_r-\delta_s$.

The functions $f_k, f^{(k')}_k$ are the «pole parts» and they are calculated according to the above-discussed algorithm. The results are

$$f_k(y,y')=\sqrt{\gamma^2-\lambda^2}\,\frac{\gamma}{N^2}\left[\frac{7}{2}+y\frac{d}{dy}+y'\frac{d}{dy'}\right]\frac{1}{yy'}\times$$

$$\times\phi_{n_r+\delta_s-1,-k}(y)\phi_{n_r-\delta_s,k}(y').$$

$$f^{(k')}_k(y,y')=\frac{\gamma}{N^2}\left[\frac{5}{2}+y\frac{d}{dy}+y'\frac{d}{dy'}-\frac{k'(\alpha Z)^2}{\gamma(k'\gamma+\lambda N)}\right]\frac{1}{yy'}\times$$

$$\times\phi_{n_r-\delta_s,k}(y)\phi_{n_r-\delta_s,k}(y')$$

Here $\phi_{n,k}(y)$ is the Sturmian function (24) of argument $y=2Zr/Na_0$. The explicit differentiation with the use of recurrence relations for Laguerre polynomials leads to the expressions for $f^{(k')}_k, f_k$ containing only the Laguerre polynomials with the same upper indices which are convenient in applications

$$f^{(k')}_k(y,y')=\frac{\gamma}{2N^2}\frac{(n_r-\delta_s)!}{\Gamma(n_r+2\lambda+\delta_s)}(yy')^{\lambda+\delta_s-1}\exp\left(-\frac{y+y'}{2}\right)\times$$

$$\times\left[\left(1-\frac{2k'(\alpha Z)^2}{\gamma(k'\gamma+\lambda N)}\right)L^{2\lambda+s}_{n_r-\delta_s}(y)L^{2\lambda+s}_{n_r-\delta_s}(y')+\right.$$

$$\left.+F_k(y)L^{2\lambda+s}_{n_r-\delta_s}(y')+L^{2\lambda+s}_{n_r-\delta_s}(y)F_k(y')\right],$$

$$f_k(y,y')=\frac{\gamma}{2N^2}\frac{n_r!}{\Gamma(n_r+2\lambda)}y^{\lambda-\delta_s}y'^{\lambda+\delta_s-1}\exp\left(-\frac{y+y'}{2}\right)\times$$

$$\times\left[3L^{2\lambda-s}_{n_r+\delta_s-1}(y)L^{2\lambda-s}_{n_r-\delta_s}(y')+L^{2\lambda-s}_{n_r+\delta_s-1}(y)F_k(y')+\right.$$

$$\left.+F_{-k}(y)L^{2\lambda+s}_{n_r-\delta_s}(y')\right].$$

Here the following abbreviation is used

$$F_k(x)=[n_r-(s-1)/2]L^{2\lambda+s}_{n_r-(s-1)/2}(x)-$$

$$-[n_r+2\lambda+(s-1)/2]L^{2\lambda+s}_{n_r-(s+3)/2}(x).$$

(ii) The matrix form of $G^{(E_{n\kappa})}_{km}(\mathbf{r},\mathbf{r}')$

The matrix structure of $G^{(E_{n\kappa})}_{km}(\mathbf{r},\mathbf{r}')$ is the same as (60)

$$G^{(E_{n\kappa})}_{km}(\mathbf{r},\mathbf{r}')=\frac{m_e}{\hbar^2a_0}\frac{2Z}{\lambda N^2}\hat{S}(k;\mathbf{n})\times$$

$$\times\begin{pmatrix}\left(h^{(11)}_k+q^{(11)}_k\right)\chi^k_m\chi^{k\dagger}_m & i\alpha Z\left(h^{(12)}_k+q^{(12)}_k\right)\chi^k_m\chi^{-k\dagger}_m\\ i\alpha Z\left(h^{(21)}_k+q^{(21)}_k\right)\chi^{-k}_m\chi^{k\dagger}_m & -\left(h^{(22)}_k+q^{(22)}_k\right)\chi^{-k}_m\chi^{-k\dagger}_m\end{pmatrix}\times$$

$$\times\hat{S}^{-1}(k;\mathbf{n}'). \qquad (78)$$

Here the «regular terms», $h^{(ij)}_k(y,y')$, are expressed in terms of functions $\tilde{g}_k,\tilde{g}_k^{(1)}$ introduced in (76):

$$h^{(11)}_k(y,y')=(k\gamma+\lambda N)\tilde{g}_\kappa(y,y'),$$

$$h^{(22)}_k(y,y')=(k\gamma-\lambda N)\tilde{g}_{-\kappa}(y,y'),$$

$$h^{(21)}_k(y,y')=\tilde{g}^{(1)}_\kappa(y,y'),\ h^{(12)}_k(y,y')=h^{(21)}_k(y',y).$$

By the similar way the «pole terms», $q^{(ij)}_k(y,y')$, involve only the functions $f_k(y,y')$ and $f^{(k')}_k(y,y')$ with $k'=\pm k$:

$$q^{(11)}_k(y,y')=(k\gamma+\lambda N)f^{(k'=k)}_\kappa(y,y'),$$

$$q^{(22)}_k(y,y')=(k\gamma-\lambda N)f^{(k'=-k)}_{-\kappa}(y,y'),$$

$$q^{(21)}_k(y,y')=f_\kappa(y,y'),\ q^{(12)}_k(y,y')=q^{(21)}_k(y,y').$$

After the linear transformations of series of Laguerre polynomials similar to eqs. (63) - (65), the expression (78) coincides with the result obtained by Swainson and Drake (1991b).

(iii) $G^{(E_{n\kappa})}_{km}(\mathbf{r},\mathbf{r}')$ *for the states with* $n_r=0$

In this case only the term with $k'=-\kappa$ in (75) should be reduced because the states with $n_r=0$ are nondegenerate in the sign of k and have fixed $k=-\kappa$. For these states we have $\gamma=\lambda$, $N=n=\kappa$ and the above results are simplified. We'll present here $G^{(E_{n_r=0})}_{km}(\mathbf{r},\mathbf{r}')$ only for the direct-products form.

At $n_r=0$ the term with $k=\kappa$ in (76) has no peculiarities and can be found directly from the general result (54) at $E=E_{n_r=0}$. The term with $k=\kappa$ after the simplest manipulations may be presented as

$$G^{(E_{n_r=0})}_{k=-\kappa,m}(\mathbf{r},\mathbf{r}')=\frac{4m_eZ}{\hbar^2a_0n}\times$$

$$\times\left[g(r,r')\theta^{(+1)}_{-\kappa,m}(\mathbf{n})\overline{\theta^{(+1)}_{-\kappa,m}(\mathbf{n}')}+\frac{\alpha Z}{2n\lambda}g^{(1)}(r,r')\sum_p p\,\theta^{(p)}_{-\kappa,m}(\mathbf{n})\overline{\theta^{(p)}_{-\kappa,m}(\mathbf{n}')}\right]$$

The function $g^{(1)}(r,r')$ arises from the term $\tilde{g}^{(1)}_{k=-\kappa}(y,y')$ in (77) at $n_r=0$ and has the form

$$g^{(1)}(r,r')=\frac{\delta(y-y')}{\sqrt{yy'}}+y^\lambda y'^{\lambda-1}\exp\left(-\frac{y+y'}{2}\right)\times$$

$$\times\sum_{p=1}^{\infty}\frac{(p-1)!L^{2\lambda+1}_{p-1}(y)L^{2\lambda-1}_p(y')}{\Gamma(p+2\lambda)}.$$

Note that the function $f_{k=-\kappa}(y,y')$ in (76) vanishes for the states with $n_r=0$ because the sum in (55) does not contain the term with $n=0$ at $k=-\kappa$.

The term $g(r,r')$, containing the «regular» and «pole» parts of radial Green function $g_{k=-\kappa}(E;r,r')$ at $E\to E_{n_r=0}$, is

$$g(r,r')=(yy')^{\lambda-1}\exp\left(-\frac{y+y'}{2}\right)\times$$

$$\times\left\{\frac{\lambda}{2n^2\Gamma(2\lambda)}\left[1+4\lambda-(\alpha Z/\lambda)^2-y-y'\right]+\right.$$

$$\left.+\sum_{p=1}^{\infty}\frac{(p-1)!L^{2\lambda-1}_p(y)L^{2\lambda-1}_p(y')}{\Gamma(2\lambda+p)}\right\},$$

In the nonrelativistic limit $(\alpha Z=0)$ we have $g^{(1)}(r,r')$, and $g(r,r')$ coincides with the nonrelativistic reduced Green function $g^{(E_n)}_l(r,r')$ for the states with $l=n$-1 (Zapriagaev *et al* 1985).

The above-presented results show, that in the second-order Dirac equation approach the radial parts of reduced (nonreduced) Green function contain only the reduced (nonreduced) functions $g_k(E;r,r')$ and $g^{(1)}_k(E;r,r')=\sqrt{1-\varepsilon^2}D(k;x)g_k(E;r,r')$ inherent the radial second-order Dirac equation.

7. Conclusion

The Dirac-Coulomb problem was solved first by the direct solution of the system of linear differential equations. The radial part of the standard solution (36) is the superposition of two Whittaker functions. Using the known recurrence relations for these functions, there are many ways to present the radial functions in terms of Whittaker functions with other indices. Actually, the second-order Dirac equation approach leads to such new forms of the Dirac-Coulomb solutions. Being based on the direct solution of the Dirac equation, these results may be derived if the «trial» function (34) to be chosed in a form similar to (45)-(50). For an example, the choice of a solution in the form

$$\Psi_{k,m}(E;\mathbf{r})=\frac{1}{r}\left[1+is\frac{\alpha Z}{\kappa+\lambda}(\gamma\cdot\mathbf{n})\right]\begin{pmatrix}u_{+1}(E;r)\chi^k_m\\ iu_{-1}(E;r)\chi^{-k}_m\end{pmatrix},$$

leads (after solving the Dirac equation for $u_{\pm1}(E;r)$) to the results obtained by Zapriagaev (1987) and Swainson and Drake (1991a). Apparently, in the present work all representations for the relativistic Coulomb Green function and wavefunctions are obtained which are most close to the nonrelativistic case, since the second-order Dirac equation approach is the natural way to generalize the nonrelativistic results on the relativistic case.

Obviously, a brief review of the Coulomb Green function history outlined in the Introduction is not complete. In particular, we did not mention the works which deal with G_E in the momentum representation. In this approach instead of the partial expansion of $G_E(\mathbf{p},\mathbf{p}')$ its expansion in αZ-powers is suitable, and the analytical calculations for small αZ are possible. This techniques was developed by Gorshkov (1964) (see also Gorshkov *et al* 1974). Moreover, for some problems, the operator representation of G_E (Le Anh Thu *et al* 1996) may be efficient. The last method is based on the connection between the problems of the four-dimensional oscillator and the hydrogen-like atom in electromagnetic fields and is an additional approach to the Coulomb problem. A certain potential for the analytical and numerical calculations of higher order matrix elements with Coulomb Green functions has a generalized Sturmian expansion (Manakov *et al* 1998). Here the radial part of Green function is presented in the form of a double series in Laguerre polinomials with two free (arbitrary) parameters α and α'. For a concrete problem, an appropriate choise of α and α' leads to a cardinal simplification in calculations of matrix elements. The results are valid both in the nonrelativistic and in the relativistic case of the squared Dirac equation.

We did not discuss in detail the nonrelativistic limits for the stated above results as they are well-known and widely used in atomic physics beginning with the pioneering work by Gavrila (1967) on the elastic scattering of photons in hydrogen atom. In the nonrelativistic case the other representations of the Coulomb Green function exist which are suitable for the concrete problems. Particularly, there are the closed form of G^{nonrel}_E in the coordinate representation (Hostler and Pratt 1963), the momentum forms (Schwinger 1964), the integral form and the Sturmian expansion of $G^{nonrel}_E(\mathbf{r},\mathbf{r}')$ in the parabolic coordinates (Manakov and Rapoport 1972). The recent review by Maquet *et al* (1998) involves a description of last results on the application of Coulomb Green functions to the concrete problems.

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