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The Dirac–Coulomb Sturmian functions in the $Z = 0$ limit: properties and applications to series expansions of the Dirac Green function and the Dirac plane wave

Radosław Szmytkowski

Atomic Physics Division, Faculty of Applied Physics and Mathematics, Technical University of Gdańsk, Narutowicza 11/12, PL 80-952 Gdańsk, Poland

E-mail: `radek@mif.pg.gda.pl`

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Abstract. Properties of the discrete Dirac–Coulomb Sturmian functions, invented recently by the author, have been investigated in the limit $Z \to 0$, where Z is a nuclear charge. Limiting forms of differential equations as well as orthogonality and closure relations obeyed by the Sturmians have been obtained. A Sturmian expansion of the radial Dirac Green function for $|E| < mc^2$ and two Sturmian expansions of the Dirac plane wave have been derived.

1. Introduction

In recent publications [1–3] we have described methods of constructing discrete [1, 3] and continuous [2] Sturmian basis sets for the first-order Dirac–Coulomb problem and discussed some properties of these functions. In [1] we have presented exemplary applications of the discrete Dirac–Coulomb Sturmians and expressed our belief in the wider range of utility of these functions. In this work we support this conviction showing further applications of the discrete relativistic Sturmian basis sets.

The paper is divided into six sections. After this introduction, in section 2 we summarize these properties of the radial Dirac–Coulomb Sturmians with $Z \neq 0$, where Z is the nuclear charge, which will be useful in later parts of the work. In section 3 we investigate the Dirac–Coulomb Sturmians in the limit $Z \to 0$ (the dependence of the relativistic Sturmians on Z is a feature distinguishing these functions from their non-relativistic counterparts [4] which are Z-independent). In section 4 we present an exemplary application of the limiting Dirac–Coulomb Sturmians and derive a series expansion of the radial Dirac Green function in the case $|E| < mc^2$. Two Dirac–Coulomb Sturmian expansions of the Dirac plane wave, analogous to the Schrödinger–Coulomb Sturmian expansion of the Helmholtz plane wave [5, 6], are derived in section 5. Remarks concluding the paper constitute section 6.

2. The radial Dirac–Coulomb Sturmians for $Z \neq 0$

The radial Dirac–Coulomb Sturmian functions $\{S_{n\kappa}(\varepsilon, 2\lambda r)\}$ and $\{T_{n\kappa}(\varepsilon, 2\lambda r)\}$ are defined [1] as non-trivial solutions to the Sturm–Liouville system consisting of the set of coupled first-order differential equations

$$\begin{pmatrix} mc^2 - E - \mu_{n\kappa}(\varepsilon)Ze^2/r & c\hbar(-\mathrm{d}/\mathrm{d}r + \kappa/r) \\ c\hbar(\mathrm{d}/\mathrm{d}r + \kappa/r) & -mc^2 - E - \mu_{n\kappa}^{-1}(\varepsilon)Ze^2/r \end{pmatrix} \begin{pmatrix} S_{n\kappa}(\varepsilon, 2\lambda r) \\ T_{n\kappa}(\varepsilon, 2\lambda r) \end{pmatrix} = 0$$

$$(0 < r < \infty) \tag{1}$$

augmented by the following boundary conditions imposed at the singular end points:

$$S_{n\kappa}(\varepsilon, 2\lambda r) \quad \text{and} \quad T_{n\kappa}(\varepsilon, 2\lambda r) \qquad \text{bounded for} \quad r \to 0 \quad \text{and} \quad r \to \infty. \tag{2}$$

In equation (1) $\mu_{n\kappa}(\varepsilon)$ is an eigenvalue parameter for the problem, m and e are the electron rest mass and the absolute value of the electronic charge, respectively, c is the speed of light, $\hbar$ is the reduced Planck constant, κ is a non-zero integer, while E and Z are fixed real parameters such that

$$0 \leqslant |E| < mc^2 \qquad 0 < \alpha|Z| < 1 \tag{3}$$

where $\alpha = e^2/c\hbar$ is the Sommerfeld fine-structure constant. For the sake of convenience, the argument of the Sturmians has been chosen as $2\lambda r$, where

$$\lambda = \frac{\sqrt{(mc^2 - E)(mc^2 + E)}}{c\hbar} \tag{4}$$

rather than r. The notation used in this work emphasizes that the Sturmians depend on the energy parameter E not only through λ but also through the parameter

$$\varepsilon = \sqrt{\frac{mc^2 - E}{mc^2 + E}}. \tag{5}$$

It is convenient to change the independent variable from r to

$$\rho = 2\lambda r \tag{6}$$

and to introduce a parameter

$$\zeta = \alpha Z. \tag{7}$$

With these changes, the eigenvalue problem constituted by equations (1) and (2) takes the form

$$\begin{pmatrix} \varepsilon/2 - \mu_{n\kappa}(\varepsilon)\,\zeta/\rho & -\mathrm{d}/\mathrm{d}\rho + \kappa/\rho \\ \mathrm{d}/\mathrm{d}\rho + \kappa/\rho & -\varepsilon^{-1}/2 - \mu_{n\kappa}^{-1}(\varepsilon)\,\zeta/\rho \end{pmatrix} \begin{pmatrix} S_{n\kappa}(\varepsilon, \rho) \\ T_{n\kappa}(\varepsilon, \rho) \end{pmatrix} = 0$$

$$(0 < \rho < \infty) \tag{8}$$

$$S_{n\kappa}(\varepsilon, \rho) \quad \text{and} \quad T_{n\kappa}(\varepsilon, \rho) \qquad \text{bounded for} \quad \rho \to 0 \quad \text{and} \quad \rho \to \infty. \tag{9}$$

It has been shown by the author [1] that there exists an infinite discrete set of eigensolutions to the problem (8) and (9). To enumerate these eigensolutions one needs positive *and* negative integer radial quantum numbers n. The eigenvalues to the problem (8) and (9) are

$$\mu_{n\kappa}(\varepsilon) = \varepsilon\zeta^{-1}(|n| + \gamma_\kappa \pm N_{n\kappa}) \qquad (n = 0, \pm 1, \pm 2, \ldots) \tag{10}$$

where

$$\gamma_\kappa = \sqrt{\kappa^2 - \zeta^2} \tag{11}$$

and

$$N_{n\kappa} = \sqrt{(|n| + \gamma_\kappa)^2 + \zeta^2} = \sqrt{|n|^2 + 2|n|\gamma_\kappa + \kappa^2} \tag{12}$$

is a so-called 'apparent principal quantum number'. Suitably normalized the upper and the lower components of the corresponding eigenfunctions are

$$S_{n\kappa}(\varepsilon,\rho) = \sqrt{\frac{\alpha(|n|+2\gamma_\kappa)|n|!}{2\varepsilon N_{n\kappa}(N_{n\kappa}\mp\kappa)\Gamma(|n|+2\gamma_\kappa)}}\rho^{\gamma_\kappa}\mathrm{e}^{-\rho/2}\left[L^{(2\gamma_\kappa)}_{|n|-1}(\rho) + \frac{\kappa\mp N_{n\kappa}}{|n|+2\gamma_\kappa}L^{(2\gamma_\kappa)}_{|n|}(\rho)\right] \tag{13}$$

$$T_{n\kappa}(\varepsilon,\rho) = \sqrt{\frac{\alpha\varepsilon(|n|+2\gamma_\kappa)|n|!}{2N_{n\kappa}(N_{n\kappa}\mp\kappa)\Gamma(|n|+2\gamma_\kappa)}}\rho^{\gamma_\kappa}\mathrm{e}^{-\rho/2}\left[L^{(2\gamma_\kappa)}_{|n|-1}(\rho) - \frac{\kappa\mp N_{n\kappa}}{|n|+2\gamma_\kappa}L^{(2\gamma_\kappa)}_{|n|}(\rho)\right] \tag{14}$$

respectively. In equations (13) and (14) $L^{(\alpha)}_n(\rho)$ denotes the generalized Laguerre polynomials defined as in [7]. (Please notice that with that definition one has $L^{(\alpha)}_{-1}(\rho) \equiv 0$, the fact of importance in the case $n = 0$). The following convention is adopted in equations (10), (13) and (14): the upper signs are to be chosen for $n > 0$ and the lower signs for $n < 0$. For $n = 0$ one chooses the upper signs if $\kappa < 0$ and the lower signs if $\kappa > 0$. In other words, one chooses the upper signs for $n \geqslant n_0(\kappa)$ and the lower signs for $n < n_0(\kappa)$, where

$$n_0(\kappa) = \begin{cases} 0 & \text{for} \quad \kappa < 0 \\ 1 & \text{for} \quad \kappa > 0. \end{cases} \tag{15}$$

The upper and the lower components of the Sturmians obey the following *two* generalized orthonormality relations:

$$\int_0^\infty \mathrm{d}\rho\, \frac{Z}{\rho}\left[\mu_{n'\kappa}(\varepsilon)\, S_{n\kappa}(\varepsilon,\rho)\, S_{n'\kappa}(\varepsilon,\rho) - \mu^{-1}_{n\kappa}(\varepsilon)\, T_{n\kappa}(\varepsilon,\rho)\, T_{n'\kappa}(\varepsilon,\rho)\right] = \delta_{nn'} \tag{16}$$

and

$$\frac{1}{2\alpha}\int_0^\infty \mathrm{d}\rho\, \left[\varepsilon S_{n\kappa}(\varepsilon,\rho)\, S_{n'\kappa}(\varepsilon,\rho) + \varepsilon^{-1}T_{n\kappa}(\varepsilon,\rho)\, T_{n'\kappa}(\varepsilon,\rho)\right] = \delta_{nn'}. \tag{17}$$

In [1, 3] we have used the properties of the generalized Laguerre polynomials to show that the Dirac–Coulomb Sturmians are complete on the real positive semi-axis $0 < \rho < \infty$. It has been shown that functions (13) and (14) satisfy the following closure relations:

$$\frac{Z}{\rho'}\sum_{n=-\infty}^{\infty}\begin{pmatrix} S_{n\kappa}(\varepsilon,\rho) \\ \mu^{-1}_{n\kappa}(\varepsilon)\, T_{n\kappa}(\varepsilon,\rho)\end{pmatrix}\begin{pmatrix} \mu_{n\kappa}(\varepsilon)\, S_{n\kappa}(\varepsilon,\rho') & -T_{n\kappa}(\varepsilon,\rho')\end{pmatrix} = \delta(\rho-\rho')\,\mathbf{1} \qquad (0 < \rho, \rho' < \infty) \tag{18}$$

and

$$\frac{1}{2\alpha}\sum_{n=-\infty}^{\infty}\begin{pmatrix} S_{n\kappa}(\varepsilon,\rho) \\ T_{n\kappa}(\varepsilon,\rho)\end{pmatrix}\begin{pmatrix} \varepsilon S_{n\kappa}(\varepsilon,\rho') & \varepsilon^{-1}T_{n\kappa}(\varepsilon,\rho')\end{pmatrix} = \delta(\rho-\rho')\,\mathbf{1} \qquad (0 < \rho, \rho' < \infty). \tag{19}$$

In equations (18) and (19) $\mathbf{1}$ denotes the unit 2×2 matrix.

3. The radial Dirac–Coulomb Sturmians in the $Z = 0$ limit

In the limiting case $Z \to 0$ from equations (11) and (12) one obtains

$$\gamma_\kappa \xrightarrow{Z\to 0} |\kappa| \tag{20}$$

$$N_{n\kappa} \xrightarrow{Z\to 0} |n| + |\kappa| \tag{21}$$

while from equation (10) one deduces

$$\mu_{n\kappa}(\varepsilon) \xrightarrow{Z\to 0^{\pm}} \begin{cases} \pm\infty & \text{for} \quad n \geqslant n_0(\kappa) \\ 0 & \text{for} \quad n < n_0(\kappa) \end{cases} \tag{22}$$

$$\mu_{n\kappa}^{-1}(\varepsilon) \xrightarrow{Z\to 0^{\pm}} \begin{cases} 0 & \text{for} \quad n \geqslant n_0(\kappa) \\ \mp\infty & \text{for} \quad n < n_0(\kappa) \end{cases} \tag{23}$$

and

$$\mu_{n\kappa}(\varepsilon)\,\zeta \xrightarrow{Z\to 0} \begin{cases} 2\varepsilon(n + |\kappa|) & \text{for} \quad n \geqslant n_0(\kappa) \\ 0 & \text{for} \quad n < n_0(\kappa) \end{cases} \tag{24}$$

$$\mu_{n\kappa}^{-1}(\varepsilon)\,\zeta \xrightarrow{Z\to 0} \begin{cases} 0 & \text{for} \quad n \geqslant n_0(\kappa) \\ -2\varepsilon^{-1}(|n| + |\kappa|) & \text{for} \quad n < n_0(\kappa). \end{cases} \tag{25}$$

The limiting forms of the radial Sturmians, derived from equations (13) and (14), are

$$S_{n\kappa}(\varepsilon, \rho) \xrightarrow{Z\to 0} \sqrt{\frac{\alpha(|n| + 2|\kappa|)|n|!}{2\varepsilon(|n| + |\kappa|)(|n| + |\kappa| \mp \kappa)\Gamma(|n| + 2|\kappa|)}} \times \rho^{|\kappa|}\mathrm{e}^{-\rho/2}\left[L_{|n|-1}^{(2|\kappa|)}(\rho) + \frac{\kappa \mp (|n| + |\kappa|)}{|n| + 2|\kappa|} L_{|n|}^{(2|\kappa|)}(\rho)\right] \tag{26}$$

and

$$T_{n\kappa}(\varepsilon, \rho) \xrightarrow{Z\to 0} \sqrt{\frac{\alpha\varepsilon(|n| + 2|\kappa|)|n|!}{2(|n| + |\kappa|)(|n| + |\kappa| \mp \kappa)\Gamma(|n| + 2|\kappa|)}} \times \rho^{|\kappa|}\mathrm{e}^{-\rho/2}\left[L_{|n|-1}^{(2|\kappa|)}(\rho) - \frac{\kappa \mp (|n| + |\kappa|)}{|n| + 2|\kappa|} L_{|n|}^{(2|\kappa|)}(\rho)\right]. \tag{27}$$

Since this should not lead to any misunderstanding, throughout the rest of the paper the limits of the functions $S_{n\kappa}(\varepsilon, \rho)$ and $T_{n\kappa}(\varepsilon, \rho)$ will be designated with $S_{n\kappa}(\varepsilon, \rho)$ and $T_{n\kappa}(\varepsilon, \rho)$, too.

In the next step we consider limits of the orthogonality and closure relations obeyed by the Sturmians. In the limit $Z \to 0$ the relation (16) splits into two relations

$$\frac{2\varepsilon}{\alpha}\int_0^\infty \mathrm{d}\rho\, \frac{n + |\kappa|}{\rho} S_{n\kappa}(\varepsilon, \rho)\, S_{n'\kappa}(\varepsilon, \rho) = \delta_{nn'} \qquad (n, n' \geqslant n_0(\kappa)) \tag{28}$$

and

$$\frac{2}{\alpha\varepsilon}\int_0^\infty \mathrm{d}\rho\, \frac{|n| + |\kappa|}{\rho} T_{n\kappa}(\varepsilon, \rho)\, T_{n'\kappa}(\varepsilon, \rho) = \delta_{nn'} \qquad (n, n' < n_0(\kappa)) \tag{29}$$

while the relation (17) formally remains unchanged

$$\frac{1}{2\alpha}\int_0^\infty \mathrm{d}\rho\, \left[\varepsilon S_{n\kappa}(\varepsilon, \rho)\, S_{n'\kappa}(\varepsilon, \rho) + \varepsilon^{-1} T_{n\kappa}(\varepsilon, \rho)\, T_{n'\kappa}(\varepsilon, \rho)\right] = \delta_{nn'}. \tag{30}$$

The closure relation (18) is modified to

$$\frac{2\varepsilon}{\alpha}\sum_{n=n_0(\kappa)}^{\infty} \frac{n + |\kappa|}{\rho'} \begin{pmatrix} S_{n\kappa}(\varepsilon, \rho) \\ 0 \end{pmatrix} \begin{pmatrix} S_{n\kappa}(\varepsilon, \rho') & 0 \end{pmatrix} + \frac{2}{\alpha\varepsilon}\sum_{n=-\infty}^{n_0(\kappa)-1} \frac{|n| + |\kappa|}{\rho'} \begin{pmatrix} 0 \\ T_{n\kappa}(\varepsilon, \rho) \end{pmatrix} \begin{pmatrix} 0 & T_{n\kappa}(\varepsilon, \rho') \end{pmatrix} = \delta(\rho - \rho')\,\mathsf{1} \qquad (0 < \rho, \rho' < \infty) \tag{31}$$

while the relation (19) formally does not undergo changes

$$\frac{1}{2\alpha}\sum_{n=-\infty}^{\infty}\begin{pmatrix} S_{n\kappa}(\varepsilon,\rho) \\ T_{n\kappa}(\varepsilon,\rho)\end{pmatrix}\begin{pmatrix}\varepsilon S_{n\kappa}(\varepsilon,\rho') & \varepsilon^{-1}T_{n\kappa}(\varepsilon,\rho')\end{pmatrix} = \delta(\rho-\rho')\,\mathbf{1}$$
$$(0 < \rho, \rho' < \infty). \tag{32}$$

To proceed further, it is convenient to consider the cases $n \geqslant n_0(\kappa)$ and $n < n_0(\kappa)$ separately. We begin with the case $n \geqslant n_0(\kappa)$. Then, from equations (8), (9), (24) and (25), one obtains that in the limit $Z \to 0$ the radial Sturmians satisfy the system

$$\begin{pmatrix} \varepsilon/2 - 2\varepsilon(n+|\kappa|)/\rho & -\mathrm{d}/\mathrm{d}\rho + \kappa/\rho \\ \mathrm{d}/\mathrm{d}\rho + \kappa/\rho & -\varepsilon^{-1}/2 \end{pmatrix}\begin{pmatrix} S_{n\kappa}(\varepsilon,\rho) \\ T_{n\kappa}(\varepsilon,\rho)\end{pmatrix} = 0$$
$$(0 < \rho < \infty;\, n \geqslant n_0(\kappa)) \tag{33}$$

$$S_{n\kappa}(\varepsilon,\rho) \quad \text{and} \quad T_{n\kappa}(\varepsilon,\rho) \qquad \text{bounded for} \quad \rho \to 0 \quad \text{and} \quad \rho \to \infty \tag{34}$$

hence, one deduces that

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}\rho^2} - \frac{\kappa(\kappa+1)}{\rho^2} + \frac{n+|\kappa|}{\rho} - \frac{1}{4}\right)S_{n\kappa}(\varepsilon,\rho) = 0 \qquad (n \geqslant n_0(\kappa)) \tag{35}$$

$$T_{n\kappa}(\varepsilon,\rho) = 2\varepsilon\left(\frac{\mathrm{d}}{\mathrm{d}\rho} + \frac{\kappa}{\rho}\right)S_{n\kappa}(\varepsilon,\rho) \qquad (n \geqslant n_0(\kappa)). \tag{36}$$

On utilizing the recurrence relations for the generalized Laguerre polynomials [7]

$$L_k^{(\alpha)}(\rho) = L_k^{(\alpha+1)}(\rho) - L_{k-1}^{(\alpha+1)}(\rho) \tag{37}$$

$$\rho L_k^{(\alpha+1)}(\rho) = (k+\alpha+1)L_k^{(\alpha)}(\rho) - (k+1)L_{k+1}^{(\alpha)}(\rho) \tag{38}$$

(the former is useful for $\kappa < 0$, the latter for $\kappa > 0$), the function $S_{n\kappa}(\varepsilon,\rho)$ may be expressed in the following compact form:

$$S_{n\kappa}(\varepsilon,\rho) = \operatorname{sgn}(\kappa)\sqrt{\frac{\alpha(n+|\kappa|-l-1)!}{2\varepsilon(n+|\kappa|)(n+|\kappa|+l)!}}\,\rho^{l+1}\mathrm{e}^{-\rho/2}L_{n+|\kappa|-l-1}^{(2l+1)}(\rho)$$
$$(n \geqslant n_0(\kappa)) \tag{39}$$

where

$$l = |\kappa + \tfrac{1}{2}| - \tfrac{1}{2} = \begin{cases} -\kappa - 1 & \text{for} \quad \kappa < 0 \\ \kappa & \text{for} \quad \kappa > 0. \end{cases} \tag{40}$$

It is evident from equation (39) that the functions $\{S_{n\kappa}(\varepsilon,\rho)\}$ possess the following symmetry property:

$$S_{n+1,l}(\varepsilon,\rho) = -S_{n,-l-1}(\varepsilon,\rho) \qquad (n \geqslant n_0(\kappa)). \tag{41}$$

It is also an immediate consequence of the closure relation (31) that

$$\frac{2\varepsilon}{\alpha}\sum_{n=n_0(\kappa)}^{\infty}\frac{n+|\kappa|}{\rho'}S_{n\kappa}(\varepsilon,\rho)\,S_{n\kappa}(\varepsilon,\rho') = \delta(\rho-\rho'). \tag{42}$$

Next we turn to considering the case $n < n_0(\kappa)$. From equations (8), (9), (24) and (25) one infers that in this case in the limit $Z \to 0$ the radial Sturmians are solutions of

$$\begin{pmatrix} \varepsilon/2 & -\mathrm{d}/\mathrm{d}\rho + \kappa/\rho \\ \mathrm{d}/\mathrm{d}\rho + \kappa/\rho & -\varepsilon^{-1}/2 + 2\varepsilon^{-1}(|n|+|\kappa|)/\rho \end{pmatrix}\begin{pmatrix} S_{n\kappa}(\varepsilon,\rho) \\ T_{n\kappa}(\varepsilon,\rho)\end{pmatrix} = 0$$
$$(0 < \rho, \rho' < \infty;\, n < n_0(\kappa)) \tag{43}$$

$$S_{n\kappa}(\varepsilon,\rho) \quad \text{and} \quad T_{n\kappa}(\varepsilon,\rho) \qquad \text{bounded for} \quad \rho\to 0 \quad \text{and} \quad \rho\to\infty \tag{44}$$

hence

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}\rho^2}-\frac{\kappa(\kappa-1)}{\rho^2}+\frac{|n|+|\kappa|}{\rho}-\frac{1}{4}\right)T_{n\kappa}(\varepsilon,\rho)=0 \qquad (n<n_0(\kappa)) \tag{45}$$

and

$$S_{n\kappa}(\varepsilon,\rho)=2\varepsilon^{-1}\left(\frac{\mathrm{d}}{\mathrm{d}\rho}-\frac{\kappa}{\rho}\right)T_{n\kappa}(\varepsilon,\rho) \qquad (n<n_0(\kappa)). \tag{46}$$

Application of the recurrence relations (37) and (38) to equation (27) yields the simplified form of the lower-component Sturmian

$$T_{n\kappa}(\varepsilon,\rho)=\operatorname{sgn}(-\kappa)\sqrt{\frac{\alpha\varepsilon(|n|+|\kappa|-l'-1)!}{2(|n|+|\kappa|)(|n|+|\kappa|+l')!}}\,\rho^{l'+1}\mathrm{e}^{-\rho/2}L^{(2l'+1)}_{|n|+|\kappa|-l'-1}(\rho) \qquad (n<n_0(\kappa)) \tag{47}$$

where

$$l'=|\kappa-\tfrac{1}{2}|-\tfrac{1}{2}=\begin{cases} l+1 & \text{for} \quad \kappa<0 \\ l-1 & \text{for} \quad \kappa>0. \end{cases} \tag{48}$$

From the closure relation (31) one infers also that

$$\frac{2}{\alpha\varepsilon}\sum_{n=-\infty}^{n_0(\kappa)-1}\frac{|n|+|\kappa|}{\rho'}T_{n\kappa}(\varepsilon,\rho)\,T_{n\kappa}(\varepsilon,\rho')=\delta(\rho-\rho'). \tag{49}$$

The closure relations (31) and (32) imply that any sufficiently regular two-component function $(\,F(r)\;\;G(r)\,)^{\mathrm{T}}$ (here and in the following the superscript T denotes a matrix transpose) defined on $0<r<\infty$ may be expanded in either of the following two ways:

$$\begin{pmatrix} F(r) \\ G(r) \end{pmatrix}=\sum_{n=-\infty}^{\infty}a_{n\kappa}(E)\begin{pmatrix} S_{n\kappa}(\varepsilon,2\lambda r) \\ T_{n\kappa}(\varepsilon,2\lambda r) \end{pmatrix} \tag{50}$$

with

$$a_{n\kappa}(E)=\frac{\lambda}{\alpha}\int_0^\infty \mathrm{d}r\,\left[\varepsilon S_{n\kappa}(\varepsilon,2\lambda r)F(r)+\varepsilon^{-1}T_{n\kappa}(\varepsilon,2\lambda r)\,G(r)\right] \tag{51}$$

or

$$\begin{pmatrix} F(r) \\ G(r) \end{pmatrix}=\sum_{n=n_0(\kappa)}^{\infty}b_{n\kappa}(E)\begin{pmatrix} S_{n\kappa}(\varepsilon,2\lambda r) \\ 0 \end{pmatrix}+\sum_{n=-\infty}^{n_0(\kappa)-1}b_{n\kappa}(E)\begin{pmatrix} 0 \\ T_{n\kappa}(\varepsilon,2\lambda r) \end{pmatrix} \tag{52}$$

with

$$b_{n\kappa}(E)=\frac{2\varepsilon}{\alpha}\int_0^\infty \mathrm{d}r\,\frac{n+|\kappa|}{r}S_{n\kappa}(\varepsilon,2\lambda r)F(r) \qquad (n\geqslant n_0(\kappa)) \tag{53}$$

$$b_{n\kappa}(E)=\frac{2}{\alpha\varepsilon}\int_0^\infty \mathrm{d}r\,\frac{|n|+|\kappa|}{r}T_{n\kappa}(\varepsilon,2\lambda r)\,G(r) \qquad (n<n_0(\kappa)). \tag{54}$$

4. Series expansion of the radial Dirac Green function for $|E| < mc^2$ in the Dirac–Coulomb Sturmian basis

As the first example of usefulness of the Dirac–Coulomb Sturmians in the $Z = 0$ limit, we shall derive a series expansion of the radial Dirac Green function $\mathsf{G}_\kappa(E, r, r')$ in the case $|E| < mc^2$.

The function $\mathsf{G}_\kappa(E, r, r')$ is a 2×2 matrix function

$$\mathsf{G}_\kappa(E, r, r') = \begin{pmatrix} G_\kappa^{(11)}(E, r, r') & G_\kappa^{(12)}(E, r, r') \\ G_\kappa^{(21)}(E, r, r') & G_\kappa^{(22)}(E, r, r') \end{pmatrix} \tag{55}$$

defined as a solution to the inhomogeneous boundary-value problem

$$\begin{pmatrix} mc^2 - E & c\hbar(-\mathrm{d}/\mathrm{d}r + \kappa/r) \\ c\hbar(\mathrm{d}/\mathrm{d}r + \kappa/r) & -mc^2 - E \end{pmatrix} \mathsf{G}_\kappa(E, r, r') = \delta(r - r')\,\mathbf{1}$$
$$(0 < r, r' < \infty;\ r' \text{ fixed};\ |E| < mc^2) \tag{56}$$

$$\mathsf{G}_\kappa(E, r, r') \qquad \text{bounded for} \quad r \to 0 \quad \text{and} \quad r \to \infty. \tag{57}$$

For notational brevity, it is convenient to make the variable transformation (6) and introduce the Green function $\mathsf{g}_\kappa(\varepsilon, \rho, \rho')$ such that

$$\mathsf{g}_\kappa(\varepsilon, \rho, \rho') = \mathsf{G}_\kappa(E, r, r'). \tag{58}$$

Obviously, $\mathsf{g}_\kappa(\varepsilon, \rho, \rho')$ is a solution of

$$\begin{pmatrix} \varepsilon/2 & -\mathrm{d}/\mathrm{d}\rho + \kappa/\rho \\ \mathrm{d}/\mathrm{d}\rho + \kappa/\rho & -\varepsilon^{-1}/2 \end{pmatrix} \mathsf{g}_\kappa(\varepsilon, \rho, \rho') = (c\hbar)^{-1}\delta(\rho - \rho')\,\mathbf{1}$$
$$(0 < \rho, \rho' < \infty;\ \rho' \text{ fixed}) \tag{59}$$

$$\mathsf{g}_\kappa(\varepsilon, \rho, \rho') \qquad \text{bounded for} \quad \rho \to 0 \quad \text{and} \quad \rho \to \infty. \tag{60}$$

The closed form of the function $\mathsf{g}_\kappa(\varepsilon, \rho, \rho')$ is known; it is

$$\begin{aligned} \mathsf{g}_\kappa(\varepsilon, \rho, \rho') = {} & \frac{2}{\pi c\hbar\varepsilon} H(\rho' - \rho) \begin{pmatrix} \hat{\imath}_l(\frac{1}{2}\rho) \\ \varepsilon\hat{\imath}_{l'}(\frac{1}{2}\rho) \end{pmatrix} \begin{pmatrix} \hat{k}_l(\frac{1}{2}\rho') & -\varepsilon\hat{k}_{l'}(\frac{1}{2}\rho') \end{pmatrix} \\ & + \frac{2}{\pi c\hbar\varepsilon} H(\rho - \rho') \begin{pmatrix} \hat{k}_l(\frac{1}{2}\rho) \\ -\varepsilon\hat{k}_{l'}(\frac{1}{2}\rho) \end{pmatrix} \begin{pmatrix} \hat{\imath}_l(\frac{1}{2}\rho') & \varepsilon\hat{\imath}_{l'}(\frac{1}{2}\rho') \end{pmatrix} \end{aligned} \tag{61}$$

where l and l' have been defined by equations (40) and (48), respectively, $\hat{\imath}_l(x)$ and $\hat{k}_l(x)$ are the modified Riccati–Bessel functions related to the modified Bessel functions [7] through

$$\hat{\imath}_l(x) = \sqrt{\tfrac{1}{2}\pi x}\, I_{l+\frac{1}{2}}(x) \qquad \hat{k}_l(x) = \sqrt{\tfrac{1}{2}\pi x}\, K_{l+\frac{1}{2}}(x) \tag{62}$$

and $H(x)$ is the Heaviside unit step function. Notice that the function $\mathsf{g}_\kappa(\varepsilon, \rho, \rho')$ possesses the symmetry property

$$\mathsf{g}_\kappa^{\mathrm{T}}(\varepsilon, \rho', \rho) = \mathsf{g}_\kappa(\varepsilon, \rho, \rho'). \tag{63}$$

We seek the Sturmian expansion of the function $\mathsf{g}_\kappa(\varepsilon, \rho, \rho')$ in the form

$$\mathsf{g}_\kappa(\varepsilon, \rho, \rho') = \sum_{n=-\infty}^{\infty} \begin{pmatrix} S_{n\kappa}(\varepsilon, \rho) \\ T_{n\kappa}(\varepsilon, \rho) \end{pmatrix} \theta_{n\kappa}^{\mathrm{T}}(\varepsilon, \rho') \tag{64}$$

where the expansion 'coefficient' $\theta^{\mathrm{T}}_{n\kappa}(\varepsilon, \rho')$ is a 1×2 matrix function of ρ'. Substitution of the expansion (64) into the differential equation (59), followed by application of equations (33) and (43), leads to

$$2\varepsilon \sum_{n=n_0(\kappa)}^{\infty} \frac{n+|\kappa|}{\rho} \begin{pmatrix} S_{n\kappa}(\varepsilon,\rho) \\ 0 \end{pmatrix} \theta^{\mathrm{T}}_{n\kappa}(\varepsilon,\rho')$$
$$-2\varepsilon^{-1} \sum_{n=-\infty}^{n_0(\kappa)-1} \frac{|n|+|\kappa|}{\rho} \begin{pmatrix} 0 \\ T_{n\kappa}(\varepsilon,\rho) \end{pmatrix} \theta^{\mathrm{T}}_{n\kappa}(\varepsilon,\rho') = (c\hbar)^{-1}\delta(\rho-\rho')\,\mathbf{1}. \tag{65}$$

To find $\theta^{\mathrm{T}}_{n\kappa}(\varepsilon, \rho')$, we multiply the above equation from the left by $\begin{pmatrix} S_{n'\kappa}(\varepsilon,\rho) & 0 \end{pmatrix}$ (with $n' \geqslant n_0(\kappa)$) or by $\begin{pmatrix} 0 & T_{n'\kappa}(\varepsilon,\rho) \end{pmatrix}$ (with $n' < n_0(\kappa)$) and integrate the results from $\rho = 0$ to ∞. By virtue of the orthogonality relations (28) and (29), this yields

$$\theta^{\mathrm{T}}_{n\kappa}(\varepsilon,\rho') = e^{-2}\begin{pmatrix} S_{n\kappa}(\varepsilon,\rho') & 0 \end{pmatrix} \qquad (n \geqslant n_0(\kappa)) \tag{66}$$

and

$$\theta^{\mathrm{T}}_{n\kappa}(\varepsilon,\rho') = -e^{-2}\begin{pmatrix} 0 & T_{n\kappa}(\varepsilon,\rho') \end{pmatrix} \qquad (n < n_0(\kappa)) \tag{67}$$

hence

$$\begin{aligned}\mathbf{g}_\kappa(\varepsilon,\rho,\rho') &= e^{-2} \sum_{n=n_0(\kappa)}^{\infty} \begin{pmatrix} S_{n\kappa}(\varepsilon,\rho) \\ T_{n\kappa}(\varepsilon,\rho) \end{pmatrix} \begin{pmatrix} S_{n\kappa}(\varepsilon,\rho') & 0 \end{pmatrix} \\ &\quad - e^{-2} \sum_{n=-\infty}^{n_0(\kappa)-1} \begin{pmatrix} S_{n\kappa}(\varepsilon,\rho) \\ T_{n\kappa}(\varepsilon,\rho) \end{pmatrix} \begin{pmatrix} 0 & T_{n\kappa}(\varepsilon,\rho') \end{pmatrix} \\ &= e^{-2} \begin{pmatrix} \sum_{n=n_0(\kappa)}^{\infty} S_{n\kappa}(\varepsilon,\rho)\,S_{n\kappa}(\varepsilon,\rho') & -\sum_{n=-\infty}^{n_0(\kappa)-1} S_{n\kappa}(\varepsilon,\rho)\,T_{n\kappa}(\varepsilon,\rho') \\ \sum_{n=n_0(\kappa)}^{\infty} T_{n\kappa}(\varepsilon,\rho)\,S_{n\kappa}(\varepsilon,\rho') & -\sum_{n=-\infty}^{n_0(\kappa)-1} T_{n\kappa}(\varepsilon,\rho)\,T_{n\kappa}(\varepsilon,\rho') \end{pmatrix}. \end{aligned} \tag{68}$$

The symmetry property (63) of the expansion (68) becomes evident after making use of the relation

$$\sum_{n=n_0(\kappa)}^{\infty} S_{n\kappa}(\varepsilon,\rho)\,T_{n\kappa}(\varepsilon,\rho') + \sum_{n=-\infty}^{n_0(\kappa)-1} S_{n\kappa}(\varepsilon,\rho)\,T_{n\kappa}(\varepsilon,\rho') = 0 \tag{69}$$

following from either of the two off-diagonal elements of the completeness equation (32).

We conclude this section by considering the non-relativistic limit of the results obtained above. For $c \to \infty$ we have $T_{n\kappa}(\varepsilon, 2\lambda r) \to 0$, which implies

$$G^{(12)}_\kappa(E,r,r') \xrightarrow{c\to\infty} 0 \qquad G^{(21)}_\kappa(E,r,r') \xrightarrow{c\to\infty} 0 \qquad G^{(22)}_\kappa(E,r,r') \xrightarrow{c\to\infty} 0. \tag{70}$$

Further, for $n \geqslant n_0(\kappa)$ from equation (39) we have

$$S_{n\kappa}(\varepsilon, 2\lambda r) \xrightarrow{c\to\infty} \begin{cases} -S_{nl}(2\overline{\lambda} r) & \text{for} \quad \kappa < 0 \\ S_{n-1,l}(2\overline{\lambda} r) & \text{for} \quad \kappa > 0 \end{cases} \tag{71}$$

where

$$S_{nl}(2\overline{\lambda} r) = \sqrt{\frac{n!}{\overline{\lambda} a_0 (n+l+1)(n+2l+1)!}}\,(2\overline{\lambda} r)^{l+1} \mathrm{e}^{-\overline{\lambda} r} L^{(2l+1)}_n(2\overline{\lambda} r) \qquad (n \geqslant 0) \tag{72}$$

with $\overline{\lambda} = \lim_{c\to\infty} \lambda$ and $a_0 = \overline{h}^2/me^2$ denoting the Bohr radius, is the non-relativistic (Z-independent) radial Schrödinger–Coulomb Sturmian function. Hence and from equation (68), we obtain

$$G_\kappa^{(11)}(E, r, r') \xrightarrow{c\to\infty} e^{-2} \sum_{n=0}^{\infty} S_{nl}(2\overline{\lambda}r)\, S_{nl}(2\overline{\lambda}r'). \tag{73}$$

The series on the right of equation (73) coincides with the Sturmian expansion of the non-relativistic free-particle radial Green function [8]

$$G_l(\overline{E}, r, r') = \frac{4m}{\pi \overline{h}^2 \overline{\lambda}} \left[\hat{\imath}_l(\overline{\lambda}r)\, \hat{k}_l(\overline{\lambda}r') H(r' - r) + \hat{k}_l(\overline{\lambda}r)\, \hat{\imath}_l(\overline{\lambda}r') H(r - r')\right] \tag{74}$$

with

$$\overline{E} = \lim_{c\to\infty} (E - mc^2) = -\frac{\overline{h}^2 \overline{\lambda}^2}{2m}. \tag{75}$$

5. Series expansions of the Dirac plane wave in the Dirac–Coulomb Sturmian bases

As the second example of the utility of the Dirac–Coulomb Sturmians in the $Z = 0$ limit, we shall construct two Sturmian expansions of the Dirac plane wave.

The free-particle time-independent Dirac equation

$$\left[-\mathrm{i}c\overline{h}\boldsymbol{\alpha} \cdot \boldsymbol{\nabla} + \beta mc^2 - \mathcal{E}\right]\Psi(\mathcal{E}, \boldsymbol{r}) = 0 \tag{76}$$

with $\Psi(\mathcal{E}, \boldsymbol{r})$ bounded,

$$|\mathcal{E}| > mc^2 \tag{77}$$

and the 4×4 Dirac matrices $\boldsymbol{\alpha}$ and β defined in terms of the 2×2 Pauli ($\boldsymbol{\sigma}$), unit ($\mathbf{1}$) and null ($\mathbf{0}$) matrices as

$$\boldsymbol{\alpha} = \begin{pmatrix} \mathbf{0} & \boldsymbol{\sigma} \\ \boldsymbol{\sigma} & \mathbf{0} \end{pmatrix} \qquad \beta = \begin{pmatrix} \mathbf{1} & \mathbf{0} \\ \mathbf{0} & -\mathbf{1} \end{pmatrix} \tag{78}$$

possesses a particular solution

$$\Psi_{\boldsymbol{k}}(\mathcal{E}, \boldsymbol{r}) = \sqrt{\frac{\mathcal{E} + mc^2}{2\mathcal{E}}} \begin{pmatrix} \chi \\ \dfrac{c\overline{h}\boldsymbol{k} \cdot \boldsymbol{\sigma}}{\mathcal{E} + mc^2} \chi \end{pmatrix} \exp(\mathrm{i}\boldsymbol{k} \cdot \boldsymbol{r}) \tag{79}$$

normalized to the unit probability density and describing a plane wave propagating in the direction $\boldsymbol{k}/k$, where $\boldsymbol{k}$ is the wavevector of modulus

$$|\boldsymbol{k}| \equiv k = \frac{\sqrt{(\mathcal{E} - mc^2)(\mathcal{E} + mc^2)}}{c\overline{h}} \tag{80}$$

while χ is a normalized ($\chi^\dagger \chi = 1$) two-component spinor describing electron spin orientation in its rest frame. It is our goal to find coefficients in the expansions

$$\Psi_{\boldsymbol{k}}(\mathcal{E},\boldsymbol{r}) = \sum_{\substack{\kappa=-\infty \\ (\kappa\neq 0)}}^{\infty} \sum_{m_j=-(|\kappa|-\frac{1}{2})}^{|\kappa|-\frac{1}{2}} \sum_{n=-\infty}^{\infty} A_{\boldsymbol{k},n\kappa m_j}(\mathcal{E},E) \frac{1}{r} \begin{pmatrix} S_{n\kappa}(\varepsilon, 2\lambda r)\,\Omega_{\kappa m_j}(\boldsymbol{r}/r) \\ \mathrm{i}T_{n\kappa}(\varepsilon, 2\lambda r)\,\Omega_{-\kappa m_j}(\boldsymbol{r}/r) \end{pmatrix} \tag{81}$$

$$\Psi_{\boldsymbol{k}}(\mathcal{E},\boldsymbol{r}) = \sum_{\substack{\kappa=-\infty \\ (\kappa\neq 0)}}^{\infty} \sum_{m_j=-(|\kappa|-\frac{1}{2})}^{|\kappa|-\frac{1}{2}} \sum_{n=n_0(\kappa)}^{\infty} B_{\boldsymbol{k},n\kappa m_j}(\mathcal{E},E) \frac{1}{r} \begin{pmatrix} S_{n\kappa}(\varepsilon, 2\lambda r)\,\Omega_{\kappa m_j}(\boldsymbol{r}/r) \\ 0 \end{pmatrix}$$
$$+ \sum_{\substack{\kappa=-\infty \\ (\kappa\neq 0)}}^{\infty} \sum_{m_j=-(|\kappa|-\frac{1}{2})}^{|\kappa|-\frac{1}{2}} \sum_{n=-\infty}^{n_0(\kappa)-1} B_{\boldsymbol{k},n\kappa m_j}(\mathcal{E},E) \frac{1}{r} \begin{pmatrix} 0 \\ \mathrm{i}T_{n\kappa}(\varepsilon, 2\lambda r)\,\Omega_{-\kappa m_j}(\boldsymbol{r}/r) \end{pmatrix} \tag{82}$$

where $\Omega_{\pm\kappa m_j}(\boldsymbol{r}/r)$ are spherical spinors. The Dirac–Coulomb Sturmian expansions (81) and (82) of the Dirac plane wave $\Psi_{\boldsymbol{k}}(\mathcal{E},\boldsymbol{r})$ are counterparts of the well known non-relativistic Schrödinger–Coulomb Sturmian expansion of the Helmholtz plane wave [5, 6].

The way we proceed is analogous to that adopted in the non-relativistic theory [5]. We expand the plane wave (79) in spherical waves [9]

$$\Psi_{\boldsymbol{k}}(\mathcal{E},\boldsymbol{r}) = \sqrt{\frac{\mathcal{E}+mc^2}{2\mathcal{E}}} \sum_{\substack{\kappa=-\infty \\ (\kappa\neq 0)}}^{\infty} \sum_{m_j=-(|\kappa|-\frac{1}{2})}^{|\kappa|-\frac{1}{2}} \frac{4\pi\mathrm{i}^l}{k} [\Omega^{\dagger}_{\kappa m_j}(\boldsymbol{k}/k)\chi] \frac{1}{r} \begin{pmatrix} P_{\kappa}(\mathcal{E},r)\,\Omega_{\kappa m_j}(\boldsymbol{r}/r) \\ \mathrm{i}Q_{\kappa}(\mathcal{E},r)\,\Omega_{-\kappa m_j}(\boldsymbol{r}/r) \end{pmatrix} \tag{83}$$

(the dagger denotes the matrix Hermitian conjugation), where the radial functions $P_{\kappa}(\mathcal{E},r)$ and $Q_{\kappa}(\mathcal{E},r)$ obey a system of coupled first-order equations

$$\begin{pmatrix} mc^2-\mathcal{E} & c\hbar(-\mathrm{d}/\mathrm{d}r+\kappa/r) \\ c\hbar(\mathrm{d}/\mathrm{d}r+\kappa/r) & -mc^2-\mathcal{E} \end{pmatrix} \begin{pmatrix} P_{\kappa}(\mathcal{E},r) \\ Q_{\kappa}(\mathcal{E},r) \end{pmatrix} = 0 \tag{84}$$

augmented by the constraints

$$P_{\kappa}(\mathcal{E},r) \quad \text{and} \quad Q_{\kappa}(\mathcal{E},r) \qquad \text{bounded for} \quad r\to 0 \quad \text{and} \quad r\to\infty. \tag{85}$$

Equation (84) may be rewritten in the form

$$P_{\kappa}(\mathcal{E},r) = \epsilon^{-1}k^{-1}\left(-\frac{\mathrm{d}}{\mathrm{d}r}+\frac{\kappa}{r}\right)Q_{\kappa}(\mathcal{E},r) \tag{86}$$

$$Q_{\kappa}(\mathcal{E},r) = \epsilon k^{-1}\left(\frac{\mathrm{d}}{\mathrm{d}r}+\frac{\kappa}{r}\right)P_{\kappa}(\mathcal{E},r) \tag{87}$$

where

$$\epsilon = \mathrm{sgn}(\mathcal{E})\sqrt{\frac{\mathcal{E}-mc^2}{\mathcal{E}+mc^2}}. \tag{88}$$

From equations (86) and (87) one finds that $P_{\kappa}(\mathcal{E},r)$ and $Q_{\kappa}(\mathcal{E},r)$ are solutions of the Riccati–Bessel equations

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}r^2}-\frac{\kappa(\kappa+1)}{r^2}+k^2\right)P_{\kappa}(\mathcal{E},r) = 0 \tag{89}$$

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}r^2}-\frac{\kappa(\kappa-1)}{r^2}+k^2\right)Q_{\kappa}(\mathcal{E},r) = 0. \tag{90}$$

Hence, with the normalization

$$P_\kappa(\mathcal{E}, r) \stackrel{r\to\infty}{\longrightarrow} \sin\left(kr - \tfrac{1}{2}\pi l\right) \tag{91}$$

one obtains

$$\begin{pmatrix} P_\kappa(\mathcal{E}, r) \\ Q_\kappa(\mathcal{E}, r) \end{pmatrix} = \begin{pmatrix} \hat{j}_l(kr) \\ \mathrm{sgn}(\kappa)\epsilon\,\hat{j}_{l'}(kr) \end{pmatrix} \tag{92}$$

where $\hat{j}_l(x)$ is the regular Riccati–Bessel function related to the Bessel function [7] through

$$\hat{j}_l(x) = \sqrt{\tfrac{1}{2}\pi x}\, J_{l+\frac{1}{2}}(x) \tag{93}$$

and the quantum numbers l and l' have been defined by equations (40) and (48), respectively.

Consider now the radial expansion

$$\begin{pmatrix} P_\kappa(\mathcal{E}, r) \\ Q_\kappa(\mathcal{E}, r) \end{pmatrix} = \sum_{n=-\infty}^{\infty} a_{n\kappa}(\mathcal{E}, E) \begin{pmatrix} S_{n\kappa}(\varepsilon, 2\lambda r) \\ T_{n\kappa}(\varepsilon, 2\lambda r) \end{pmatrix}. \tag{94}$$

In accord with equations (50) and (51), the expansion coefficients $\{a_{n\kappa}(\mathcal{E}, E)\}$ are given by

$$a_{n\kappa}(\mathcal{E}, E) = \frac{\lambda}{\alpha}\int_0^\infty \mathrm{d}r\,\left[\varepsilon S_{n\kappa}(\varepsilon, 2\lambda r) P_\kappa(\mathcal{E}, r) + \varepsilon^{-1} T_{n\kappa}(\varepsilon, 2\lambda r) Q_\kappa(\mathcal{E}, r)\right]. \tag{95}$$

It is clear that once the coefficients $\{a_{n\kappa}(\mathcal{E}, E)\}$ have been found, the coefficients $\{A_{\boldsymbol{k},n\kappa m_j}(\mathcal{E}, E)\}$ are also known since equations (81), (83) and (94) imply

$$A_{\boldsymbol{k},n\kappa m_j}(\mathcal{E}, E) = \sqrt{\frac{\mathcal{E} + mc^2}{2\mathcal{E}}}\,\frac{4\pi \mathrm{i}^l}{k}\left[\Omega^\dagger_{\kappa m_j}(\boldsymbol{k}/k)\chi\right] a_{n\kappa}(\mathcal{E}, E). \tag{96}$$

To evaluate the coefficients $\{a_{n\kappa}(\mathcal{E}, E)\}$ we simplify the integral on the right of equation (95) by utilizing the properties of the Sturmians and the functions $P_\kappa(\mathcal{E}, r)$ and $Q_\kappa(\mathcal{E}, r)$. At first let us discuss the case when $n \geqslant n_0(\kappa)$. Then, employing equations (36) and (87), one finds

$$\begin{aligned}\int_0^\infty \mathrm{d}r\, T_{n\kappa}(\varepsilon, 2\lambda r) Q_\kappa(\mathcal{E}, r) &= \epsilon k^{-1}\varepsilon\lambda^{-1}\int_0^\infty \mathrm{d}r\left[\left(\frac{\mathrm{d}}{\mathrm{d}r} + \frac{\kappa}{r}\right) S_{n\kappa}(\varepsilon, 2\lambda r)\right]\left[\left(\frac{\mathrm{d}}{\mathrm{d}r} + \frac{\kappa}{r}\right) P_\kappa(\mathcal{E}, r)\right] \\ &\quad (n \geqslant n_0(\kappa))\end{aligned} \tag{97}$$

which, after integration by parts transferring the operator acting on $S_{n\kappa}(\varepsilon, 2\lambda r)$ to the right and after making use of equation (89), is transformed into

$$\int_0^\infty \mathrm{d}r\, T_{n\kappa}(\varepsilon, 2\lambda r) Q_\kappa(\mathcal{E}, r) = \epsilon k\varepsilon\lambda^{-1}\int_0^\infty \mathrm{d}r\, S_{n\kappa}(\varepsilon, 2\lambda r) P_\kappa(\mathcal{E}, r) \qquad (n \geqslant n_0(\kappa)). \tag{98}$$

Substitution of the result (98) into equation (95) yields

$$a_{n\kappa}(\mathcal{E}, E) = \frac{\epsilon k + \varepsilon\lambda}{\alpha}\int_0^\infty \mathrm{d}r\, S_{n\kappa}(\varepsilon, 2\lambda r) P_\kappa(\mathcal{E}, r) \qquad (n \geqslant n_0(\kappa)). \tag{99}$$

Consider next the case $n < n_0(\kappa)$. This time it is convenient to transform the first part of the integral in equation (95). Upon utilizing equations (46) and (86), integrating by parts and using equation (90), we obtain

$$\int_0^\infty \mathrm{d}r\, S_{n\kappa}(\varepsilon, 2\lambda r) P_\kappa(\varepsilon, r) = -\epsilon^{-1}k\varepsilon^{-1}\lambda^{-1}\int_0^\infty \mathrm{d}r\, T_{n\kappa}(\varepsilon, 2\lambda r) Q_\kappa(\mathcal{E}, r) \qquad (n < n_0(\kappa)). \tag{100}$$

Employing the result (100) in equation (95) and making use of the identity

$$\epsilon^{-1}k - \varepsilon^{-1}\lambda = \epsilon k + \varepsilon\lambda \tag{101}$$

yields

$$a_{n\kappa}(\mathcal{E}, E) = -\frac{\epsilon k + \varepsilon\lambda}{\alpha}\int_0^\infty \mathrm{d}r\, T_{n\kappa}(\varepsilon, 2\lambda r) Q_\kappa(\mathcal{E}, r) \qquad (n < n_0(\kappa)). \tag{102}$$

It remains to evaluate the integrals in equations (99) and (102). Upon utilizing equations (39), (47) and (92), one has

$$a_{n\kappa}(\mathcal{E}, E) = \mathrm{sgn}(\kappa)(\epsilon k + \varepsilon\lambda)\sqrt{\frac{(n + |\kappa| - l - 1)!}{2\alpha\varepsilon(n + |\kappa|)(n + |\kappa| + l)!}}\, I_{n+|\kappa|-l-1,l}(k, \lambda) \qquad (n \geqslant n_0(\kappa)) \tag{103}$$

and

$$a_{n\kappa}(\mathcal{E}, E) = \epsilon(\epsilon k + \varepsilon\lambda)\sqrt{\frac{\varepsilon(|n| + |\kappa| - l' - 1)!}{2\alpha(|n| + |\kappa|)(|n| + |\kappa| + l')!}}\, I_{|n|+|\kappa|-l'-1,l'}(k, \lambda) \qquad (n < n_0(\kappa)) \tag{104}$$

where

$$I_{nl}(k, \lambda) = \int_0^\infty \mathrm{d}r\, (2\lambda r)^{l+1}\mathrm{e}^{-\lambda r} L_n^{(2l+1)}(2\lambda r)\, \hat{j}_l(kr). \tag{105}$$

The integral $I_{nl}(k, \lambda)$ was evaluated by Podolsky and Pauling [10] (cf also [5]) who considered the Schrödinger–Coulomb problem in the momentum representation. They obtained

$$I_{nl}(k, \lambda) = 2^{2l+2} l!(n + l + 1)\frac{k^{l+1}\lambda^{l+2}}{(k^2 + \lambda^2)^{l+2}} C_n^{(l+1)}\left(\frac{k^2 - \lambda^2}{k^2 + \lambda^2}\right) \tag{106}$$

where $C_n^{(\alpha)}(x)$ is the Gegenbauer polynomial [7]. With this result, we finally arrive at

$$a_{n\kappa}(\mathcal{E}, E) = \mathrm{sgn}(\kappa)\, 2^{2l+3/2} l!\sqrt{\frac{(n + |\kappa|)(n + |\kappa| - l - 1)!}{\alpha\varepsilon(n + |\kappa| + l)!}} \times(\epsilon k + \varepsilon\lambda)\frac{k^{l+1}\lambda^{l+2}}{(k^2 + \lambda^2)^{l+2}} C_{n+|\kappa|-l-1}^{(l+1)}\left(\frac{k^2 - \lambda^2}{k^2 + \lambda^2}\right) \qquad (n \geqslant n_0(\kappa)) \tag{107}$$

and

$$a_{n\kappa}(\mathcal{E}, E) = 2^{2l'+3/2} l'!\sqrt{\frac{\varepsilon(|n| + |\kappa|)(|n| + |\kappa| - l' - 1)!}{\alpha(|n| + |\kappa| + l')!}} \times\epsilon(\epsilon k + \varepsilon\lambda)\frac{k^{l'+1}\lambda^{l'+2}}{(k^2 + \lambda^2)^{l'+2}} C_{|n|+|\kappa|-l'-1}^{(l'+1)}\left(\frac{k^2 - \lambda^2}{k^2 + \lambda^2}\right) \qquad (n < n_0(\kappa)). \tag{108}$$

Equations (96), (107) and (108) solve the problem of constructing the Sturmian expansion (81).

It is interesting to consider the non-relativistic limit of the expansion (94). Denoting $\overline{\lambda} = \lim_{c\to\infty}\lambda$ and $\overline{k} = \lim_{c\to\infty} k$, equations (107) and (108) yield

$$a_{n\kappa}(\mathcal{E}, E) \xrightarrow{c\to\infty} \mathrm{sgn}(\kappa)\, 2^{2l+1} l!\sqrt{\frac{\overline{\lambda} a_0(n + |\kappa|)(n + |\kappa| - l - 1)!}{(n + |\kappa| + l)!}} \times\left(\frac{\overline{k}\,\overline{\lambda}}{\overline{k}^2 + \overline{\lambda}^2}\right)^{l+1} C_{n+|\kappa|-l-1}^{(l+1)}\left(\frac{\overline{k}^2 - \overline{\lambda}^2}{\overline{k}^2 + \overline{\lambda}^2}\right) \qquad (n \geqslant n_0(\kappa)) \tag{109}$$

and

$$a_{n\kappa}(\mathcal{E}, E) \xrightarrow{c\to\infty} 0 \qquad (n < n_0(\kappa)). \tag{110}$$

On combining the non-relativistic limits of equations (39), (92) and (94) with equations (109) and (110), one arrives at the well known expansion of the Riccati–Bessel function in the Laguerre polynomials basis [11, 12]

$$\hat{j}_l(\bar{k}r) = \sum_{n=0}^{\infty} \frac{2^{2l+1} l! n!}{(n+2l+1)!} \left(\frac{\bar{k}\,\bar{\lambda}}{\bar{k}^2 + \bar{\lambda}^2}\right)^{l+1} C_n^{(l+1)}\left(\frac{\bar{k}^2 - \bar{\lambda}^2}{\bar{k}^2 + \bar{\lambda}^2}\right)(2\bar{\lambda}r)^{l+1} \mathrm{e}^{-\bar{\lambda}r} L_n^{(2l+1)}(2\bar{\lambda}r). \tag{111}$$

Consider next the radial expansion

$$\begin{pmatrix} P_\kappa(\mathcal{E}, r) \\ Q_\kappa(\mathcal{E}, r) \end{pmatrix} = \sum_{n=n_0(\kappa)}^{\infty} b_{n\kappa}(\mathcal{E}, E) \begin{pmatrix} S_{n\kappa}(\varepsilon, 2\lambda r) \\ 0 \end{pmatrix} + \sum_{n=-\infty}^{n_0(\kappa)-1} b_{n\kappa}(\mathcal{E}, E) \begin{pmatrix} 0 \\ T_{n\kappa}(\varepsilon, 2\lambda r) \end{pmatrix}. \tag{112}$$

Knowledge of the coefficients $\{b_{n\kappa}(\mathcal{E}, E)\}$ implies knowledge of the coefficients $\{B_{\boldsymbol{k},n\kappa m_j}(\mathcal{E}, E)\}$, since equations (82), (83) and (112) give

$$B_{\boldsymbol{k},n\kappa m_j}(\mathcal{E}, E) = \sqrt{\frac{\mathcal{E} + mc^2}{2\mathcal{E}}} \frac{4\pi \mathrm{i}^l}{k} \left[\Omega^\dagger_{\kappa m_j}(\boldsymbol{k}/k)\chi\right] b_{n\kappa}(\mathcal{E}, E). \tag{113}$$

Based on equations (52)–(54) we find that the expansion coefficients $\{b_{n\kappa}(\mathcal{E}, E)\}$ are given by

$$b_{n\kappa}(\mathcal{E}, E) = \frac{2\varepsilon}{\alpha} \int_0^\infty \mathrm{d}r\, \frac{n + |\kappa|}{r} S_{n\kappa}(\varepsilon, 2\lambda r) P_\kappa(\mathcal{E}, r) \qquad (n \geqslant n_0(\kappa)) \tag{114}$$

$$b_{n\kappa}(\mathcal{E}, E) = \frac{2}{\alpha\varepsilon} \int_0^\infty \mathrm{d}r\, \frac{|n| + |\kappa|}{r} T_{n\kappa}(\varepsilon, 2\lambda r) Q_\kappa(\mathcal{E}, r) \qquad (n < n_0(\kappa)). \tag{115}$$

It appears that the integrals in equations (114) and (115) may be expressed in terms of the integrals occurring in equations (99) and (102), respectively. To show this, let us premultiply equation (35) by $P_\kappa(\mathcal{E}, r)$, equation (45) by $Q_\kappa(\mathcal{E}, r)$ and integrate the results from $r = 0$ to ∞. This yields

$$\int_0^\infty \mathrm{d}r\, P_\kappa(\mathcal{E}, r)\left(\frac{\mathrm{d}^2}{\mathrm{d}r^2} - \frac{\kappa(\kappa+1)}{r^2} + \frac{2\lambda(n + |\kappa|)}{r} - \lambda^2\right) S_{n\kappa}(\varepsilon, 2\lambda r) = 0 \qquad (n \geqslant n_0(\kappa)) \tag{116}$$

and

$$\int_0^\infty \mathrm{d}r\, Q_\kappa(\mathcal{E}, r)\left(\frac{\mathrm{d}^2}{\mathrm{d}r^2} - \frac{\kappa(\kappa-1)}{r^2} + \frac{2\lambda(|n| + |\kappa|)}{r} - \lambda^2\right) T_{n\kappa}(\varepsilon, 2\lambda r) = 0 \qquad (n < n_0(\kappa)). \tag{117}$$

Integrating by parts twice and transferring in this way the action of the operators in parentheses to the left, after utilizing the differential equations (89) and (90) we obtain

$$\int_0^\infty \mathrm{d}r\, \left(-k^2 - \lambda^2 + \frac{2\lambda(n + |\kappa|)}{r}\right) P_\kappa(\mathcal{E}, r)\, S_{n\kappa}(\varepsilon, 2\lambda r) = 0 \qquad (n \geqslant n_0(\kappa)) \tag{118}$$

and

$$\int_0^\infty \mathrm{d}r\, \left(-k^2 - \lambda^2 + \frac{2\lambda(|n| + |\kappa|)}{r}\right) Q_\kappa(\mathcal{E}, r)\, T_{n\kappa}(\varepsilon, 2\lambda r) = 0 \qquad (n < n_0(\kappa)) \tag{119}$$

hence, it follows that

$$\int_0^\infty \mathrm{d}r\, \frac{n+|\kappa|}{r} S_{n\kappa}(\varepsilon, 2\lambda r) P_\kappa(\mathcal{E}, r) = \frac{k^2+\lambda^2}{2\lambda} \int_0^\infty \mathrm{d}r\, S_{n\kappa}(\varepsilon, 2\lambda r) P_\kappa(\mathcal{E}, r) \qquad (n \geqslant n_0(\kappa)) \tag{120}$$

and

$$\int_0^\infty \mathrm{d}r\, \frac{|n|+|\kappa|}{r} T_{n\kappa}(\varepsilon, 2\lambda r) Q_\kappa(\mathcal{E}, r) = \frac{k^2+\lambda^2}{2\lambda} \int_0^\infty \mathrm{d}r\, T_{n\kappa}(\varepsilon, 2\lambda r) Q_\kappa(\mathcal{E}, r) \qquad (n < n_0(\kappa)). \tag{121}$$

Consequently, from equations (99), (102), (114), (115), (120) and (121) we deduce the following relationships between the coefficients $\{b_{n\kappa}(\mathcal{E}, E)\}$ and $\{a_{n\kappa}(\mathcal{E}, E)\}$:

$$b_{n\kappa}(\mathcal{E}, E) = \frac{\varepsilon(k^2+\lambda^2)}{\lambda(\epsilon k + \varepsilon\lambda)} a_{n\kappa}(\mathcal{E}, E) \qquad (n \geqslant n_0(\kappa)) \tag{122}$$

$$b_{n\kappa}(\mathcal{E}, E) = -\frac{k^2+\lambda^2}{\varepsilon\lambda(\epsilon k + \varepsilon\lambda)} a_{n\kappa}(\mathcal{E}, E) \qquad (n < n_0(\kappa)). \tag{123}$$

Inserting here the results (107) and (108), we conclude that

$$b_{n\kappa}(\mathcal{E}, E) = \mathrm{sgn}(\kappa)\, 2^{2l+3/2} l! \sqrt{\frac{\varepsilon(n+|\kappa|)(n+|\kappa|-l-1)!}{\alpha(n+|\kappa|+l)!}} \times \left(\frac{k\lambda}{k^2+\lambda^2}\right)^{l+1} C^{(l+1)}_{n+|\kappa|-l-1}\left(\frac{k^2-\lambda^2}{k^2+\lambda^2}\right) \qquad (n \geqslant n_0(\kappa)) \tag{124}$$

and

$$b_{n\kappa}(\mathcal{E}, E) = -2^{2l'+3/2} l'! \sqrt{\frac{(|n|+|\kappa|)(|n|+|\kappa|-l'-1)!}{\alpha\varepsilon(|n|+|\kappa|+l')!}} \times \epsilon \left(\frac{k\lambda}{k^2+\lambda^2}\right)^{l'+1} C^{(l'+1)}_{|n|+|\kappa|-l'-1}\left(\frac{k^2-\lambda^2}{k^2+\lambda^2}\right) \qquad (n < n_0(\kappa)). \tag{125}$$

Equations (113), (124) and (125) constitute the solution to the problem of constructing the Sturmian expansion (82). Since

$$b_{n\kappa}(\mathcal{E}, E) \xrightarrow{c\to\infty} a_{n\kappa}(\mathcal{E}, E) \qquad (n \geqslant n_0(\kappa)) \tag{126}$$

in the non-relativistic limit the upper component of the radial expansion (112) brings on the Laguerre expansion (111).

6. Conclusions

In this work we have investigated properties of the Dirac–Coulomb Sturmians in the $Z = 0$ limit. To illustrate the utility of the results obtained, a series expansion of the Dirac Green function for $|E| < mc^2$ and two series expansions of the Dirac plane wave have been derived. The latter expansions are relativistic counterparts of the Schrödinger–Coulomb Sturmian expansion of the Helmholtz plane wave which in recent years found applications in non-relativistic quantum physics [5, 6].

It is worth emphasizing that the results of section 5 open the way to a presentation of the relativistic generalization of the J-matrix theory of scattering on short-range potentials [11, 13, 14]. To consider the relativistic J-matrix theory of scattering on potentials vanishing like the Coulomb potential [11] one needs a Dirac–Coulomb Sturmian expansion of the Dirac–Coulomb wave. Currently we are working on deriving such an expansion.

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