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The continuum Schrödinger–Coulomb and Dirac–Coulomb Sturmian functions

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Abstract. Spherical continuum Sturmian functions for the Schrödinger–Coulomb and Dirac–Coulomb problems are constructed by solving appropriate Sturm–Liouville systems. It is proved that in the non-relativistic case a spectrum of potential strengths is continuous and covers the whole real axis. In the relativistic case two Sturmian sets may be derived. For the relativistic Sturm–Liouville problems their eigenvalue spectra consist of the real axes with zero excluded plus circumferences in the complex plane centred at zero. It is shown that, as a consequence of a relationship existing between the two families of the continuum Dirac–Coulomb Sturmians, each family obeys two orthogonality and two closure relations.

1. Introduction

In theoretical analysis of atomic and molecular phenomena one frequently uses various functional basis sets for representing wave or Green functions of a particular physical system in forms of series or integral expansions (for a comprehensive review, see [1]). Although in principle any complete set may be used for this purpose, it is well known that for particular applications some basis sets are more suitable than others. On physical grounds it is expected, and experience confirms these expectations, that adequate functions may be frequently generated by solving an eigenvalue problem consisting of some solvable time-independent model wave equation, with structure reflecting the main physical features of a system considered, plus appropriate boundary conditions. Usually, in such problems one chooses energy as an eigenvalue and functions generated in that way are called 'energy eigenfunctions'. In some cases, however, it may be more profitable to obtain a basis in an alternative way by treating the energy E as a fixed parameter and introduce an eigenvalue parameter in some other place in the wave equation. Functions generated in that manner are generally referred to as 'Sturmian functions' [2, 3].

Among a variety of Sturmian basis sets which may be obtained by making different choices of wave equations and eigenvalue parameters, Coulomb Sturmian functions are of particular value because of the exceptional role played in atomic physics by the Coulomb problem (cf [2–4] and references therein). In the non-relativistic case they are solutions of the Schrödinger–Coulomb wave equation with a fixed value of the energy parameter, augmented by appropriate boundary conditions, and with the strength of the Coulomb potential chosen as an eigenvalue. (In the relativistic case the Dirac–Coulomb Sturmians have to be defined in a more involved way, cf [4] and sections 4 and 5 of this work.) It is known [3, 5, 6] that two different types of the Coulomb Sturmian functions may be constructed according to the domain from which the energy parameter E is chosen. In the non-relativistic case, if $E < 0$, it appears that the Schrödinger–Coulomb Sturmians form a discrete set [2, 3]. Properties of the discrete Sturmians have been thoroughly investigated and the functions are widely used in atomic physics (for a comprehensive bibliography, see [2, 4]). In contrast, studies concerning the Schrödinger–Coulomb Sturmians for which $E > 0$ are scarce. Searching through the literature we found that the problem of constructing non-relativistic positive-energy Coulomb Sturmian states was considered, very briefly, by Khristenko [3], Blinder [5, 6] and more recently, in a different way, by Ovchinnikov and Macek [7]. Khristenko [3] defined positive-energy Sturmian functions as those solutions of the Schrödinger–Coulomb equation with $E > 0$ which, after multiplication by the radius r, remained bounded for $0 \leqslant r \leqslant \infty$. He found that the spectrum of potential strengths was continuous and covered the whole real axis. In two works concerning Sturmian propagators for the non-relativistic attractive Coulomb problem Blinder [5, 6] postulated the same form of the positive-energy Schrödinger–Coulomb Sturmians as had been found before by Khristenko but, in disagreement with Khristenko's results, claimed that the spectrum of potential strengths was limited to the positive real half-axis.

A different approach to the problem was proposed by Ovchinnikov and Macek [7]. In a work concerning positive-energy Sturmians for *two*-Coulomb-centre problems these authors defined the non-relativistic *one*-centre positive-energy Coulomb Sturmian states, as those solutions of the Schrödinger–Coulomb wave equation with $E > 0$ which were regular at the origin and behaved as purely outgoing waves for $r \to \infty$. Functions defined in that manner are analytic continuation of the negative-energy Sturmians to the positive-energy domain. The potential-strength spectrum for this problem was found to be discrete and purely imaginary. The Sturmians obtained in that way possess, however, a deficiency owing to a long-range nature of the Coulomb field: they become unbounded as r increases to infinity. For that reason, in spite of claims to the contrary [7], Ovchinnikov and Macek's Sturmians fail to obey a simple orthogonality relation and it is difficult to infer anything about the completeness of this set.

We have found the situation to be unsatisfactory and decided to reinvestigate the subject. Because of the difficulty encountered by the method of Ovchinnikov and Macek, in this work we have adopted the approach of Khristenko. We present a method of construction of a set of the non-relativistic positive-energy (or *continuum*) Schrödinger–Coulomb Sturmians and discuss their basic properties. It is shown that the spectrum of potential-strength eigenvalues coincides with the *whole* real axis. This resolves the disagreement between Khristenko's and Blinder's results in Khristenko's favour. We also discuss important problems concerning orthogonality and normalization of the positive-energy Schrödinger–Coulomb Sturmians.

In recent years one observes a rapid growth of interest in developing mathematical tools suitable for the use in relativistic theoretical atomic physics [8, 9]. Therefore, it is natural to ask whether it would be possible to find a relativistic analogue of the continuum Schrödinger–Coulomb Sturmians: the continuum Dirac–Coulomb Sturmian functions. Such a set (or sets) should be useful in the analysis of those atomic continuum processes where the relativity is expected to play an important role. We have studied the subject in a manner similar to that used in our study of discrete Dirac–Coulomb Sturmians [4] and found that the answer is positive: by solving suitable boundary-value problems with a fixed value of the energy parameter selected so that $|E| > mc^2$ and with cleverly chosen eigenvalues it is possible to construct *two* different sets of continuum Dirac–Coulomb Sturmian functions. A detailed analysis of properties of these functions, presented in sections 4 and 5, leads to the conclusion that the eigenvalue spectrum for each problem is continuous and consists of the real axis with zero excluded, plus a circumference in the complex plane centred at zero.

It is also found that, as a consequence of a relationship existing between the two sets of the relativistic continuum Sturmians, both functional sets obey *two* orthogonality and *two* closure relations.

2. The continuum Schrödinger–Coulomb Sturmian functions

We define the three-dimensional continuum Schrödinger–Coulomb Sturmian functions $\{\Phi_{\mu_l l m_l}(E, \boldsymbol{r})\}$ as simultaneous eigenfunctions of the orbital angular momentum operators

$$\boldsymbol{\Lambda}^2 = -[\boldsymbol{r} \times \boldsymbol{\nabla}]^2 \qquad \Lambda_z = -\mathrm{i}\left[x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right] \tag{1}$$

with quantum numbers $l(l+1)$ and m_l, respectively, satisfying an eigenvalue problem consisting of the Schrödinger–Coulomb differential equation

$$\left[-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2 - \mu_l\frac{Ze^2}{r} - E\right]\Phi_{\mu_l l m_l}(E, \boldsymbol{r}) = 0 \tag{2}$$

and the boundary conditions

$$r\Phi_{\mu_l l m_l}(E, \boldsymbol{r}) \overset{r\to 0}{\sim} r^{l+1} \qquad r\Phi_{\mu_l l m_l}(E, \boldsymbol{r}) \text{ bounded for } r \to \infty. \tag{3}$$

Here $E > 0$ and Z are fixed real parameters and μ_l is an eigenvalue for the problem. Since the Sturmians are eigenfunctions of $\boldsymbol{\Lambda}^2$ and Λ_z, they are of the form

$$\Phi_{\mu_l l m_l}(E, \boldsymbol{r}) = \frac{1}{r}S_{\mu_l l}(2\lambda r)Y_{l m_l}(\boldsymbol{n}) \tag{4}$$

where $\boldsymbol{n} = \boldsymbol{r}/r$ is the unit vector directed along $\boldsymbol{r}$ and $\{Y_{l m_l}(\boldsymbol{n})\}$ are normalized spherical harmonics. The functions $\{S_{\mu_l l}(2\lambda r)\}$ are the radial continuum Schrödinger–Coulomb Sturmians and are non-trivial solutions of the Sturm–Liouville problem

$$\left[-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}r^2} + \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2} - \mu_l\frac{Ze^2}{r} - E\right]S_{\mu_l l}(2\lambda r) = 0 \qquad (0 \leqslant r < \infty) \tag{5}$$

$$S_{\mu_l l}(2\lambda r) \overset{l}{\sim} r \to 0 r^{l+1} \qquad S_{\mu_l l}(2\lambda r) \text{ bounded for } r \to \infty \tag{6}$$

which may be obtained in the standard way after substitution of the functions (4) into equations (2) and (3). For the sake of convenience, we have chosen the argument of $S_{\mu_l l}$ as $2\lambda r$, where

$$\lambda = \sqrt{\frac{2mE}{\hbar^2}} \tag{7}$$

rather than r. Since $E > 0$, the parameter λ is real and positive. In this section it will be our primary aim to find the explicit form of the radial functions $\{S_{\mu_l l}(2\lambda r)\}$ and to investigate their properties.

To accomplish this aim, we change the independent variable to

$$x = 2\lambda r \tag{8}$$

and rewrite the Sturm–Liouville problem (5) and (6) in the form

$$\left[\frac{\mathrm{d}^2}{\mathrm{d}x^2} - \frac{\left(l+\frac{1}{2}\right)^2 - \frac{1}{4}}{x^2} + \frac{\eta_l}{x} + \frac{1}{4}\right]S_{\mu_l l}(x) = 0 \qquad (0 \leqslant x < \infty) \tag{9}$$

$$S_{\mu_l l}(x) \overset{x\to 0}{\sim} x^{l+1} \qquad S_{\mu_l l}(x) \text{ bounded for } x \to \infty \tag{10}$$

with η_l defined as

$$\eta_l = \mu_l \frac{Zme^2}{\hbar^2\lambda} \qquad \left(= \mu_l \frac{Z}{\lambda a_0}\right) \tag{11}$$

where a_0 is the Bohr radius. Equation (9) resembles the Whittaker differential equation [10, 11], the only difference between the two equations being in the sign in front of $\frac{1}{4}$. The difference vanishes if one changes the differentiation variable from x to $\mathrm{i}x$. With this transformation equation (9) becomes

$$\left[\frac{\mathrm{d}^2}{\mathrm{d}(\mathrm{i}x)^2} - \frac{(l+\frac{1}{2})^2 - \frac{1}{4}}{(\mathrm{i}x)^2} + \frac{-\mathrm{i}\eta_l}{\mathrm{i}x} - \frac{1}{4}\right] S_{\mu_l l}(x) = 0. \tag{12}$$

A solution to this equation which satisfies the boundary condition imposed on $S_{\mu_l l}(x)$ at $x = 0$ is [10]

$$\tilde{S}_{\mu_l l}(x) = A_{\mu_l l} M_{-\mathrm{i}\eta_l, l+1/2}(\mathrm{i}x) \tag{13}$$

where $M_{\eta\gamma}(x)$ is the Whittaker function of the first kind and $A_{\mu_l l}$ is a normalization factor. The tilde indicates that so far we have taken care of the boundary condition at the origin but not of the one at infinity.

We now ask the question: for what values of the parameter μ_l is the function $\tilde{S}_{\mu_l l}(x)$ defined by equation (13) bounded for $x \to \infty$? To answer this question we utilize the expansion (193) obtaining the asymptotic form of the function $\tilde{S}_{\mu_l l}(x)$

$$\tilde{S}_{\mu_l l}(x) \stackrel{x\to\infty}{\longrightarrow} \frac{1}{2\mathrm{i}} B^{(+)}_{\mu_l l} \exp[\mathrm{i}(\tfrac{1}{2}x + \eta_l \ln x - \tfrac{1}{2}\pi l - \sigma_l(\eta_l))] \\ - \frac{1}{2\mathrm{i}} B^{(-)}_{\mu_l l} \exp[-\mathrm{i}(\tfrac{1}{2}x + \eta_l \ln x - \tfrac{1}{2}\pi l + \sigma_l(-\eta_l))] \tag{14}$$

where

$$B^{(\pm)}_{\mu_l l} = \frac{2\mathrm{i}^{l+1}\mathrm{e}^{-\pi\eta_l/2}\Gamma(2l+2)}{|\Gamma(l+1\pm\mathrm{i}\eta_l)|} A_{\mu_l l} \tag{15}$$

and $\sigma_\gamma(\pm\eta)$ is the Coulomb phase shift defined as

$$\sigma_\gamma(\pm\eta) = \arg\Gamma(\gamma + 1 \pm \mathrm{i}\eta) \tag{16}$$

(complex values of η are also admitted in equation (16)). It is evident from equation (14) that the function $\tilde{S}_{\mu_l l}(x)$ remains bounded for $x \to \infty$ as long as the parameter η_l is real (for, if $\mathrm{Im}\,\eta_l \neq 0$ then $\tilde{S}_{\mu_l l}(x)$ diverges for $x \to \infty$ as $x^{|\mathrm{Im}\,\eta_l|}$). In view of the relationship (11) and the assumptions made concerning E and Z, this implies that the Sturm–Liouville problem (9) and (10) (or, equivalently, (5) and (6)) has a continuous spectrum of real eigenvalues

$$-\infty < \mu_l < +\infty. \tag{17}$$

It is clear from the above considerations that there is a one-to-one correspondence between the eigenfunctions $S_{\mu_l l}(x)$ and the eigenvalues μ_l, i.e. for fixed l the eigenvalues μ_l are non-degenerate. Since the range of the eigenvalues μ_l is the same for all l, henceforth we shall omit the subscript l at μ_l and η_l.

The result (17) dissolves, in Khristenko's favour, the discrepancy between the result found by that author [3], who concluded that the spectrum of μ-eigenvalues covered the whole real axis, and the result obtained by Blinder [5, 6], who claimed that the spectrum was restricted to the real positive half-axis.

The reality of η may be exploited to simplify the asymptotic expression (14). It follows from the definition (16) and the well known properties of the Euler gamma function [10] that for real η and γ one has

$$|\Gamma(\gamma+1+\mathrm{i}\eta)| = |\Gamma(\gamma+1-\mathrm{i}\eta)| \qquad \sigma_\gamma(-\eta) = -\sigma_\gamma(\eta). \tag{18}$$

Hence and from equation (14) one infers that

$$S_{\mu l}(x) \stackrel{x\to\infty}{\longrightarrow} B_{\mu l}\sin\left(\tfrac{1}{2}x + \eta\ln x - \tfrac{1}{2}\pi l - \sigma_l(\eta)\right) \tag{19}$$

where

$$B_{\mu l} = \frac{2\mathrm{i}^{l+1}\mathrm{e}^{-\pi\eta/2}\Gamma(2l+2)}{|\Gamma(l+1+\mathrm{i}\eta)|}A_{\mu l}. \tag{20}$$

We shall now consider a problem of orthogonality and normalization of the radial Sturmians $S_{\mu l}(x)$ constructed above. Since we have encountered continuum spectrum, the problem is more subtle than in the case of negative-energy discrete Sturmians [2]. Initially, we consider two solutions to the boundary-value problem (9) and (10), $S_{\mu l}(x')$ and $S_{\mu' l}(x')$, corresponding to eigenvalues μ and μ', respectively. Premultiplying the equation satisfied by $S_{\mu l}(x')$ by $S_{\mu' l}(x')$ and vice versa, subtracting the results, integrating from $x' = 0$ to $x' = x$ and utilizing the boundary condition at $x' = 0$ we obtain

$$(\eta - \eta')\int_0^x \mathrm{d}x'\,\frac{1}{x'}S_{\mu l}(x')S_{\mu' l}(x') = S_{\mu l}(x)\frac{\mathrm{d}S_{\mu' l}(x)}{\mathrm{d}x} - S_{\mu' l}(x)\frac{\mathrm{d}S_{\mu l}(x)}{\mathrm{d}x} \tag{21}$$

where

$$\eta' = \mu'\,\frac{Z}{\lambda a_0}. \tag{22}$$

If x is sufficiently large, we may replace the Sturmians on the right-hand side by their asymptotic forms (19). After some simple algebra one obtains

$$\int_0^x \mathrm{d}x'\,\frac{1}{x'}S_{\mu l}(x')S_{\mu' l}(x') \stackrel{x\to\infty}{\longrightarrow} \frac{1}{2}B_{\mu l}B_{\mu' l}\frac{\sin[(\eta-\eta')\ln x - (\sigma_l(\eta) - \sigma_l(\eta'))]}{\eta - \eta'}. \tag{23}$$

In the limit $x \to \infty$ the fraction on the right-hand side tends to one of the well known representations of the Dirac delta function $\delta(\eta - \eta')$ times π [13], so that

$$\int_0^\infty \mathrm{d}x\,\frac{1}{x}S_{\mu l}(x)S_{\mu' l}(x) = \frac{\pi}{2}B_{\mu l}^2\delta(\eta - \eta'). \tag{24}$$

We find it convenient to normalize the radial Sturmians according to

$$\int_0^\infty \mathrm{d}x\,\frac{|Z|}{x}S_{\mu l}(x)S_{\mu' l}(x) = \delta(\mu - \mu'). \tag{25}$$

If we choose $B_{\mu l}$ to be positive, equation (11) and condition (25) yield

$$B_{\mu l} = \sqrt{\frac{2}{\pi\lambda a_0}}. \tag{26}$$

Hence and from equation (20) it follows that

$$A_{\mu l} = \frac{\mathrm{e}^{\pi\eta/2}}{\mathrm{i}^{l+1}\sqrt{2\pi\lambda a_0}}\frac{|\Gamma(l+1+\mathrm{i}\eta)|}{\Gamma(2l+2)}. \tag{27}$$

Consequently, the radial continuum Schrödinger–Coulomb Sturmian functions normalized according to equation (25) are given by

$$S_{\mu l}(x) = \frac{\mathrm{e}^{\pi\eta/2}}{\mathrm{i}^{l+1}\sqrt{2\pi\lambda a_0}}\frac{|\Gamma(l+1+\mathrm{i}\eta)|}{\Gamma(2l+2)}M_{-\mathrm{i}\eta,l+1/2}(\mathrm{i}x). \tag{28}$$

An equivalent form of the radial Sturmians

$$S_{\mu l}(x) = \frac{\mathrm{i}^{l+1}\mathrm{e}^{\pi\eta/2}}{\sqrt{2\pi\lambda a_0}} \frac{|\Gamma(l+1+\mathrm{i}\eta)|}{\Gamma(2l+2)} M_{\mathrm{i}\eta,l+1/2}(-\mathrm{i}x) \tag{29}$$

is obtained if in equation (28) one makes use of the Kummer transformation (197). It may be easily verified by utilizing any of equations (28) and (29) and the complex conjugation relation (198) that the radial functions $\{S_{\mu l}(x)\}$ are real.

Since the radial functions $\{S_{\mu l}(x)\}$ are eigenfunctions of the Hermitian Sturm–Liouville problem, they form a complete set. On multiplying both sides of equation (25) by $S_{\mu l}(x')$, integrating over the complete spectrum of μ-eigenvalues, interchanging the order of integrations over μ and x and making use of fundamental properties of the Dirac delta function we obtain

$$\int_0^\infty \mathrm{d}x\, S_{\mu' l}(x) \frac{|Z|}{x} \int_{-\infty}^\infty \mathrm{d}\mu S_{\mu l}(x) S_{\mu l}(x') = S_{\mu' l}(x'). \tag{30}$$

Hence, a closure relation

$$\frac{|Z|}{x'} \int_{-\infty}^\infty \mathrm{d}\mu\, S_{\mu l}(x) S_{\mu l}(x') = \delta(x - x') \tag{31}$$

follows.

Once the radial Sturmians $\{S_{\mu l}(2\lambda r)\}$ are known, the three-dimensional Sturmians $\{\Phi_{\mu l m_l}(E, \boldsymbol{r})\}$ may be found in accord with equation (4). Moreover, the following orthogonality

$$\int_{\mathcal{R}^3} \mathrm{d}^3\boldsymbol{r}\, \frac{|Z|}{r} \Phi^*_{\mu l m_l}(E, \boldsymbol{r}) \Phi_{\mu' l' m'_l}(E, \boldsymbol{r}) = \delta(\mu - \mu') \delta_{ll'} \delta_{m_l m'_l} \tag{32}$$

and closure

$$\frac{|Z|}{r'} \sum_{l m_l} \int_{-\infty}^\infty \mathrm{d}\mu\, \Phi_{\mu l m_l}(E, \boldsymbol{r}) \Phi^*_{\mu l m_l}(E, \boldsymbol{r}') = \delta(\boldsymbol{r} - \boldsymbol{r}') \tag{33}$$

relations for the functions $\{\Phi_{\mu l m_l}(E, \boldsymbol{r})\}$ are readily deduced from equations (4), (25) and (31) and from the well known properties of the spherical harmonics. Throughout the paper the asterisk denotes the complex conjugation.

In appendix B we briefly discuss an important difference between the continuum Coulomb and non-Coulomb Sturmian functions.

3. Expansions in terms of the continuum Schrödinger–Coulomb Sturmian functions

Any sufficiently regular function $F(x)$ defined on the real positive half-axis $0 \leqslant x < \infty$ may be represented as an integral involving the radial Sturmians $\{S_{\mu l}(x)\}$ in the following manner

$$F(x) = \int_{-\infty}^\infty \mathrm{d}\mu\, \chi_{\mu l} S_{\mu l}(x) \tag{34}$$

where the function $\chi_{\mu l}$ is determined from the orthogonality relation (25) to be

$$\chi_{\mu l} = \int_0^\infty \mathrm{d}x\, \frac{|Z|}{x} S_{\mu l}(x) F(x). \tag{35}$$

The function $\chi_{\mu l}$ may be called a 'Coulomb Sturmian transform' of the function $F(x)$.

In the three-dimensional case, any sufficiently regular function $\Psi(\boldsymbol{r})$ has a Sturmian representation

$$\Psi(\boldsymbol{r}) = \sum_{lm_l} \int_{-\infty}^{\infty} \mathrm{d}\mu\, \chi_{\mu l m_l} \Phi_{\mu l m_l}(E, \boldsymbol{r}). \tag{36}$$

The transform function $\chi_{\mu l m_l}$ may be found from the latter equation by premultiplying it with $r^{-1}|Z|\Phi^*_{\mu' l' m_l'}(E, \boldsymbol{r})$ and integrating the result over $\mathcal{R}^3$. Utilizing the orthogonality relation (32) and omitting the primes yields

$$\chi_{\mu l m_l} = \int_{\mathcal{R}^3} \mathrm{d}^3\boldsymbol{r}\, \frac{|Z|}{r}\, \Phi^*_{\mu l m_l}(E, \boldsymbol{r}) \Psi(\boldsymbol{r}). \tag{37}$$

4. The continuum Dirac–Coulomb Sturmian functions of the first kind

Let $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ be a vector constructed from the Pauli matrices and let I be the unit 2×2 matrix. We introduce the 4×4 matrices

$$\boldsymbol{\alpha} = \begin{pmatrix} 0 & \boldsymbol{\sigma} \\ \boldsymbol{\sigma} & 0 \end{pmatrix} \qquad \beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix} \qquad \boldsymbol{\Sigma} = \begin{pmatrix} \boldsymbol{\sigma} & 0 \\ 0 & \boldsymbol{\sigma} \end{pmatrix} \qquad \mathcal{I} = \begin{pmatrix} I & 0 \\ 0 & I \end{pmatrix} \tag{38}$$

and the operators

$$\mathcal{K} = -\beta(\boldsymbol{\Sigma} \cdot \boldsymbol{\Lambda} + \mathcal{I}) \qquad \boldsymbol{\Lambda} = -\mathrm{i}\boldsymbol{r} \times \boldsymbol{\nabla}. \tag{39}$$

The four-component continuum Dirac–Coulomb Sturmian functions of the first kind, $\{\Phi_{\mu_\kappa \kappa m_j}(E, \boldsymbol{r})\}$, are defined as those simultaneous eigenfunctions of the operators $\mathcal{K}$ and $J_z = \Lambda_z + \frac{1}{2}\Sigma_z$, with the respective eigenvalues κ and m_j, which are solutions of the boundary-value problem consisting of the set of four coupled first-order partial differential equations

$$\left[-\mathrm{i}c\hbar\boldsymbol{\alpha} \cdot \boldsymbol{\nabla} + \beta mc^2 - E\mathcal{I} - \mathcal{M}_\kappa \frac{Ze^2}{r}\right] \Phi_{\mu_\kappa \kappa m_j}(E, \boldsymbol{r}) = 0 \tag{40}$$

augmented by boundary conditions

$$r\Phi_{\mu_\kappa \kappa m_j}(E, \boldsymbol{r}) \overset{l}{\sim} r \to 0 r^{\gamma_\kappa} \qquad r\Phi_{\mu_\kappa \kappa m_j}(E, \boldsymbol{r}) \text{ bounded for } r \to \infty. \tag{41}$$

Here E and Z are fixed real parameters such that

$$|E| > mc^2 \qquad 0 < \alpha|Z| < 1 \tag{42}$$

$\alpha = e^2/c\hbar$ (not to be confused with the matrix $\boldsymbol{\alpha}$) is the Sommerfeld fine structure constant, the exponent γ_κ is defined by

$$\gamma_\kappa = +\sqrt{\kappa^2 - (\alpha Z)^2} \tag{43}$$

$\mathcal{M}_\kappa$ is the 4×4 matrix of the form

$$\mathcal{M}_\kappa = \begin{pmatrix} \mu_\kappa I & 0 \\ 0 & \mu_\kappa^{-1} I \end{pmatrix} \tag{44}$$

and μ_κ is an eigenvalue for the problem (40) and (41). The boundary conditions (41) are to be understood in the sense that any of the four components of $r\Phi_{\mu_\kappa \kappa m_j}(E, \boldsymbol{r})$ vanishes like r^{γ_κ} for $r \to 0$ and is bounded for $r \to \infty$.

A brief comment is in order here. The boundary condition imposed on the Sturmians in the vicinity of $r = 0$ is chosen to be identical with the one obeyed there by the Dirac–Coulomb wave functions of the same angular symmetry. It was shown by Drake and

Goldman [14] that it is this choice that demands the unusual way in which the eigenvalue μ_κ enters equation (40).

Since the Sturmians are eigenfunctions of the operators $\mathcal{K}$ and J_z, they have the form

$$\Phi_{\mu_\kappa \kappa m_j}(E, \boldsymbol{r}) = \frac{1}{r} \begin{pmatrix} S_{\mu_\kappa \kappa}(2\lambda r)\Omega_{\kappa m_j}(\boldsymbol{n}) \\ \mathrm{i}T_{\mu_\kappa \kappa}(2\lambda r)\Omega_{-\kappa m_j}(\boldsymbol{n}) \end{pmatrix} \tag{45}$$

where $\{S_{\mu_\kappa \kappa}(2\lambda r)\}$ and $\{T_{\mu_\kappa \kappa}(2\lambda r)\}$ are the radial continuum Dirac–Coulomb Sturmians, $\boldsymbol{n} = \boldsymbol{r}/r$ is the unit vector along $\boldsymbol{r}$ and $\{\Omega_{\pm\kappa m_j}(\boldsymbol{n})\}$ are spherical spinors. The parameter λ entering the argument of the Sturmians is defined as

$$\lambda = \frac{\sqrt{(E - mc^2)(E + mc^2)}}{c\hbar} \tag{46}$$

and in the non-relativistic limit it converges to the quantity defined by equation (7). We notice also that, since $|E| > mc^2$, the parameter λ is real and positive. After substitution of the function (45) into equations (40) and (41), the angular part of the problem may be separated out in the standard way [15] and one finds that the radial Sturmians are non-trivial solutions to the Sturm–Liouville problem

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

$$(0 \leqslant r < \infty) \tag{47}$$

$$S_{\mu_\kappa \kappa}(2\lambda r) \overset{l}{\sim} r \to 0 r^{\gamma_\kappa} \qquad T_{\mu_\kappa \kappa}(2\lambda r) \overset{l}{\sim} r \to 0 r^{\gamma_\kappa} \tag{48}$$

$$S_{\mu_\kappa \kappa}(2\lambda r) \text{ and } T_{\mu_\kappa \kappa}(2\lambda r) \text{ bounded for } r \to \infty. \tag{49}$$

It is convenient to change the independent variable by the transformation

$$x = 2\lambda r \tag{50}$$

and introduce parameters

$$\varepsilon = \sqrt{\frac{E - mc^2}{E + mc^2}} \qquad \zeta = \alpha Z. \tag{51}$$

With this transformation, equations (47)–(49) become

$$\begin{pmatrix} -\varepsilon/2 - \mu_\kappa \zeta/x & -\mathrm{d}/\mathrm{d}x + \kappa/x \\ \mathrm{d}/\mathrm{d}x + \kappa/x & -\varepsilon^{-1}/2 - \mu_\kappa^{-1}\zeta/x \end{pmatrix} \begin{pmatrix} S_{\mu_\kappa \kappa}(x) \\ T_{\mu_\kappa \kappa}(x) \end{pmatrix} = 0 \qquad (0 \leqslant x < \infty) \tag{52}$$

$$S_{\mu_\kappa \kappa}(x) \overset{x\to 0}{\sim} x^{\gamma_\kappa} \qquad T_{\mu_\kappa \kappa}(x) \overset{x\to 0}{\sim} x^{\gamma_\kappa} \tag{53}$$

$$S_{\mu_\kappa \kappa}(x) \text{ and } T_{\mu_\kappa \kappa}(x) \text{ bounded for } x \to \infty. \tag{54}$$

To find the explicit form of the radial Dirac–Coulomb Sturmians and their eigenvalues we rewrite equation (52) in the form

$$\frac{\mathrm{d}S_{\mu_\kappa \kappa}(x)}{\mathrm{d}x} + \frac{\kappa}{x} S_{\mu_\kappa \kappa}(x) - \left(\frac{1}{2}\varepsilon^{-1} + \mu_\kappa^{-1}\frac{\zeta}{x}\right) T_{\mu_\kappa \kappa}(x) = 0 \tag{55}$$

$$\frac{\mathrm{d}T_{\mu_\kappa \kappa}(x)}{\mathrm{d}x} - \frac{\kappa}{x} T_{\mu_\kappa \kappa}(x) + \left(\frac{1}{2}\varepsilon + \mu_\kappa \frac{\zeta}{x}\right) S_{\mu_\kappa \kappa}(x) = 0. \tag{56}$$

We shall solve this system following the method proposed by Kolsrud [16]. Differentiation of both equations with respect to x followed by elimination of the first derivatives yields a system of two coupled second-order differential equations

$$\left[\frac{\mathrm{d}^2}{\mathrm{d}x^2} - \frac{\gamma_\kappa^2}{x^2} + \frac{\eta_\kappa}{x} + \frac{1}{4}\right] \begin{pmatrix} S_\kappa(x) \\ T_\kappa(x) \end{pmatrix} + \frac{\mathcal{C}_\kappa}{x^2} \begin{pmatrix} S_\kappa(x) \\ T_\kappa(x) \end{pmatrix} = 0 \tag{57}$$

where

$$\eta_\kappa = \tfrac{1}{2}\zeta\left(\varepsilon^{-1}\mu_\kappa + \varepsilon\mu_\kappa^{-1}\right) \tag{58}$$

and

$$\mathcal{C}_\kappa = \begin{pmatrix} -\kappa & \mu_\kappa^{-1}\zeta \\ -\mu_\kappa\zeta & \kappa \end{pmatrix}. \tag{59}$$

Equations (57) may be decoupled by a similarity transformation that diagonalizes $\mathcal{C}_\kappa$

$$\mathcal{B}_\kappa = \mathcal{A}_\kappa^{-1}\mathcal{C}_\kappa\mathcal{A}_\kappa. \tag{60}$$

The spectral matrix $\mathcal{B}_\kappa$ and the modal matrix $\mathcal{A}_\kappa$ are

$$\mathcal{B}_\kappa = \begin{pmatrix} -\gamma_\kappa & 0 \\ 0 & \gamma_\kappa \end{pmatrix} \tag{61}$$

$$\mathcal{A}_\kappa = \begin{pmatrix} 1 & \mu_\kappa^{-1}\zeta^{-1}(\kappa-\gamma_\kappa) \\ \mu_\kappa\zeta^{-1}(\kappa-\gamma_\kappa) & 1 \end{pmatrix}. \tag{62}$$

Denoting

$$\begin{pmatrix} F_{\mu_\kappa\kappa}(x) \\ G_{\mu_\kappa\kappa}(x) \end{pmatrix} = \mathcal{A}_\kappa^{-1}\begin{pmatrix} S_{\mu_\kappa\kappa}(x) \\ T_{\mu_\kappa\kappa}(x) \end{pmatrix} \tag{63}$$

we rewrite equation (57) in the form

$$\left[\frac{\mathrm{d}^2}{\mathrm{d}x^2} - \frac{\left(\gamma_\kappa+\frac{1}{2}\right)^2-\frac{1}{4}}{x^2} + \frac{\eta_\kappa}{x} + \frac{1}{4}\right]F_{\mu_\kappa\kappa}(x) = 0 \tag{64}$$

$$\left[\frac{\mathrm{d}^2}{\mathrm{d}x^2} - \frac{\left(\gamma_\kappa-\frac{1}{2}\right)^2-\frac{1}{4}}{x^2} + \frac{\eta_\kappa}{x} + \frac{1}{4}\right]G_{\mu_\kappa\kappa}(x) = 0. \tag{65}$$

As in the non-relativistic case discussed in section 2, it is convenient to change the differentiation variable from x to $\mathrm{i}x$. This yields a pair of Whittaker equations

$$\left[\frac{\mathrm{d}^2}{\mathrm{d}(\mathrm{i}x)^2} - \frac{\left(\gamma_\kappa+\frac{1}{2}\right)^2-\frac{1}{4}}{(\mathrm{i}x)^2} + \frac{-\mathrm{i}\eta_\kappa}{\mathrm{i}x} - \frac{1}{4}\right]F_{\mu_\kappa\kappa}(x) = 0 \tag{66}$$

$$\left[\frac{\mathrm{d}^2}{\mathrm{d}(\mathrm{i}x)^2} - \frac{\left(\gamma_\kappa-\frac{1}{2}\right)^2-\frac{1}{4}}{(\mathrm{i}x)^2} + \frac{-\mathrm{i}\eta_\kappa}{\mathrm{i}x} - \frac{1}{4}\right]G_{\mu_\kappa\kappa}(x) = 0. \tag{67}$$

Their solutions regular at $x = 0$ are [10, 11]

$$F_{\mu_\kappa\kappa}(x) = A_{\mu_\kappa\kappa}M_{-\mathrm{i}\eta_\kappa,\gamma_\kappa+1/2}(\mathrm{i}x) \tag{68}$$

$$G_{\mu_\kappa\kappa}(x) = B_{\mu_\kappa\kappa}M_{-\mathrm{i}\eta_\kappa,\gamma_\kappa-1/2}(\mathrm{i}x) \tag{69}$$

where $A_{\mu_\kappa\kappa}$ and $B_{\mu_\kappa\kappa}$ are constants independent on x. Hence, on utilizing equations (62) and (63), we find

$$\tilde{S}_{\mu_\kappa\kappa}(x) = A_{\mu_\kappa\kappa}M_{-\mathrm{i}\eta_\kappa,\gamma_\kappa+1/2}(\mathrm{i}x) + B_{\mu_\kappa\kappa}\mu_\kappa^{-1}\zeta^{-1}(\kappa-\gamma_\kappa)M_{-\mathrm{i}\eta_\kappa,\gamma_\kappa-1/2}(\mathrm{i}x) \tag{70}$$

$$\tilde{T}_{\mu_\kappa\kappa}(x) = A_{\mu_\kappa\kappa}\mu_\kappa\zeta^{-1}(\kappa-\gamma_\kappa)M_{-\mathrm{i}\eta_\kappa,\gamma_\kappa+1/2}(\mathrm{i}x) + B_{\mu_\kappa\kappa}M_{-\mathrm{i}\eta_\kappa,\gamma_\kappa-1/2}(\mathrm{i}x). \tag{71}$$

The tilde indicates that so far we have ignored the boundary condition imposed on the functions $S_{\mu_\kappa\kappa}(x)$ and $T_{\mu_\kappa\kappa}(x)$ at the infinity. Since the functions $\tilde{S}_{\mu_\kappa\kappa}(x)$ and $\tilde{T}_{\mu_\kappa\kappa}(x)$ are solutions of the pair of coupled first-order differential equations (55) and (56), the ratio of the constants $A_{\mu_\kappa\kappa}$ and $B_{\mu_\kappa\kappa}$ is fixed. Substituting equations (70) and (71) into equation (55) we obtain

$$\frac{A_{\mu_\kappa\kappa}}{B_{\mu_\kappa\kappa}} = -\mu_\kappa^{-1}\zeta^{-1}(\kappa-\gamma_\kappa) \times \frac{\mathrm{i}M'_{-\mathrm{i}\eta_\kappa,\gamma_\kappa-1/2}(\mathrm{i}x) - (\gamma_\kappa/x)M_{-\mathrm{i}\eta_\kappa,\gamma_\kappa-1/2}(\mathrm{i}x) - \frac{1}{2}\varepsilon^{-1}\mu_\kappa\zeta^{-1}(\kappa+\gamma_\kappa)M_{-\mathrm{i}\eta_\kappa,\gamma_\kappa-1/2}(\mathrm{i}x)}{\mathrm{i}M'_{-\mathrm{i}\eta_\kappa,\gamma_\kappa+1/2}(\mathrm{i}x) + (\gamma_\kappa/x)M_{-\mathrm{i}\eta_\kappa,\gamma_\kappa+1/2}(\mathrm{i}x) - \frac{1}{2}\varepsilon^{-1}\mu_\kappa\zeta^{-1}(\kappa-\gamma_\kappa)M_{-\mathrm{i}\eta_\kappa,\gamma_\kappa+1/2}(\mathrm{i}x)} \tag{72}$$

where the prime denotes differentiation with respect to the *argument*. Since the left-hand side of equation (72) is independent of x, the same must be true for the right-hand side and we may choose the value of x in this equation at our convenience. Choosing $x = 0$ and making use of the limiting relation (192) we obtain

$$\frac{A_{\mu_\kappa\kappa}}{B_{\mu_\kappa\kappa}} = -\mathrm{i}\mu_\kappa^{-1}\zeta^{-1}\frac{\eta_\kappa\kappa+\xi_\kappa\gamma_\kappa}{2\gamma_\kappa(2\gamma_\kappa+1)} \tag{73}$$

where

$$\xi_\kappa = \tfrac{1}{2}\zeta\left(\varepsilon^{-1}\mu_\kappa - \varepsilon\mu_\kappa^{-1}\right). \tag{74}$$

The parameters η_κ, ξ_κ, κ and γ_κ are related by

$$\eta_\kappa^2 - \xi_\kappa^2 = \zeta^2 = \kappa^2 - \gamma_\kappa^2. \tag{75}$$

On applying equation (73) we find

$$\tilde{S}_{\mu_\kappa\kappa}(x) = C_{\mu_\kappa\kappa}\left[M_{-\mathrm{i}\eta_\kappa,\gamma_\kappa-1/2}(\mathrm{i}x) - \mathrm{i}\frac{\eta_\kappa\kappa+\xi_\kappa\gamma_\kappa}{2\gamma_\kappa(2\gamma_\kappa+1)(\kappa-\gamma_\kappa)}M_{-\mathrm{i}\eta_\kappa,\gamma_\kappa+1/2}(\mathrm{i}x)\right] \tag{76}$$

$$\tilde{T}_{\mu_\kappa\kappa}(x) = \varepsilon C_{\mu_\kappa\kappa}\frac{\kappa+\gamma_\kappa}{\eta_\kappa-\xi_\kappa}\left[M_{-\mathrm{i}\eta_\kappa,\gamma_\kappa-1/2}(\mathrm{i}x) - \mathrm{i}\frac{\eta_\kappa\kappa+\xi_\kappa\gamma_\kappa}{2\gamma_\kappa(2\gamma_\kappa+1)(\kappa+\gamma_\kappa)}M_{-\mathrm{i}\eta_\kappa,\gamma_\kappa+1/2}(\mathrm{i}x)\right] \tag{77}$$

where $C_{\mu_\kappa\kappa}$ is a multiplicative constant factor. It appears that functions (76) and (77) may be rewritten in forms more suitable for applications by using recurrence relations obeyed by the Whittaker function. Making use of equations (199) and (200) we obtain

$$\tilde{S}_{\mu_\kappa\kappa}(x) = \frac{1}{2}C_{\mu_\kappa\kappa}(\mathrm{i}x)^{-1/2}\Bigg[\left(1-\mathrm{i}\frac{\kappa+\gamma_\kappa}{\eta_\kappa-\xi_\kappa}\right)M_{-\mathrm{i}\eta_\kappa-1/2,\gamma_\kappa}(\mathrm{i}x) + \left(1+\mathrm{i}\frac{\kappa+\gamma_\kappa}{\eta_\kappa-\xi_\kappa}\right)M_{-\mathrm{i}\eta_\kappa+1/2,\gamma_\kappa}(\mathrm{i}x)\Bigg] \tag{78}$$

$$\tilde{T}_{\mu_\kappa\kappa}(x) = \frac{1}{2}\mathrm{i}\varepsilon C_{\mu_\kappa\kappa}(\mathrm{i}x)^{-1/2}\Bigg[\left(1-\mathrm{i}\frac{\kappa+\gamma_\kappa}{\eta_\kappa-\xi_\kappa}\right)M_{-\mathrm{i}\eta_\kappa-1/2,\gamma_\kappa}(\mathrm{i}x) - \left(1+\mathrm{i}\frac{\kappa+\gamma_\kappa}{\eta_\kappa-\xi_\kappa}\right)M_{-\mathrm{i}\eta_\kappa+1/2,\gamma_\kappa}(\mathrm{i}x)\Bigg]. \tag{79}$$

In the following we shall need asymptotic forms of $\tilde{S}_{\mu_\kappa\kappa}(x)$ and $\tilde{T}_{\mu_\kappa\kappa}(x)$ for large values of x. Such forms are readily obtained by utilizing equations (78) and (79) and the asymptotic expansion (193). One finds

$$\tilde{S}_{\mu_\kappa\kappa}(x) \stackrel{x\to\infty}{\longrightarrow} \tfrac{1}{2}D^{(+)}_{\mu_\kappa\kappa}\exp[\mathrm{i}(\tfrac{1}{2}x+\eta_\kappa\ln x-\tfrac{1}{2}\pi\gamma_\kappa-\sigma_{\gamma_\kappa}(\eta_\kappa)-\phi^{(+)}_\kappa)] + \tfrac{1}{2}D^{(-)}_{\mu_\kappa\kappa}\exp[-\mathrm{i}(\tfrac{1}{2}x+\eta_\kappa\ln x-\tfrac{1}{2}\pi\gamma_\kappa+\sigma_{\gamma_\kappa}(-\eta_\kappa)-\phi^{(-)}_\kappa)] \tag{80}$$

$$\tilde{T}_{\mu_\kappa\kappa}(x) \stackrel{x\to\infty}{\longrightarrow} \tfrac{1}{2}\mathrm{i}\varepsilon D^{(+)}_{\mu_\kappa\kappa}\exp[\mathrm{i}(\tfrac{1}{2}x+\eta_\kappa\ln x-\tfrac{1}{2}\pi\gamma_\kappa-\sigma_{\gamma_\kappa}(\eta_\kappa)-\phi^{(+)}_\kappa)] - \tfrac{1}{2}\mathrm{i}\varepsilon D^{(-)}_{\mu_\kappa\kappa}\exp[-\mathrm{i}(\tfrac{1}{2}x+\eta_\kappa\ln x-\tfrac{1}{2}\pi\gamma_\kappa+\sigma_{\gamma_\kappa}(-\eta_\kappa)-\phi^{(-)}_\kappa)] \tag{81}$$

where $D^{(\pm)}_{\mu_\kappa\kappa}$ are multiplicative factors related to $C_{\mu_\kappa\kappa}$ by

$$D^{(\pm)}_{\mu_\kappa\kappa} = \left|1 \mp \mathrm{i}\frac{\kappa+\gamma_\kappa}{\eta_\kappa-\xi_\kappa}\right| \frac{\Gamma(2\gamma_\kappa+1)\mathrm{e}^{(\mathrm{i}\gamma_\kappa-\eta_\kappa)\pi/2}}{|\Gamma(\gamma_\kappa+1\pm\mathrm{i}\eta_\kappa)|} C_{\mu_\kappa\kappa} \tag{82}$$

while

$$\phi^{(\pm)}_\kappa = \mp \arg\left(1 \mp \mathrm{i}\frac{\kappa+\gamma_\kappa}{\eta_\kappa-\xi_\kappa}\right). \tag{83}$$

The Coulomb phase $\sigma_\gamma(\eta)$ has been defined by equation (16).

We are now in a position to find the spectrum of the Sturm–Liouville problem (52)–(54). We ask: for what values of the parameter μ_κ are the functions $\tilde{S}_{\mu_\kappa\kappa}(x)$ and $\tilde{T}_{\mu_\kappa\kappa}(x)$ bounded for $x \to \infty$? It is evident from equations (80) and (81) that this happens if and only if the parameter η_κ premultiplying $\ln x$ in the arguments of the exponential functions is real (otherwise, if $\mathrm{Im}\,\eta_\kappa \neq 0$, the functions $\tilde{S}_{\mu_\kappa\kappa}(x)$ and $\tilde{T}_{\mu_\kappa\kappa}(x)$ diverge asymptotically as $x^{|\mathrm{Im}\,\eta_\kappa|}$). Allowing for complex values of μ_κ, we may rewrite equation (58) in the form

$$\eta_\kappa = \tfrac{1}{2}\zeta\varepsilon^{-1}|\mu_\kappa|^{-2}[(|\mu_\kappa|^2+\varepsilon^2)\mathrm{Re}\,\mu_\kappa + \mathrm{i}(|\mu_\kappa|^2-\varepsilon^2)\mathrm{Im}\,\mu_\kappa]. \tag{84}$$

We see that the condition

$$\mathrm{Im}\,\eta_\kappa = 0 \tag{85}$$

is equivalent to

$$\mathrm{Im}\,\mu_\kappa = 0 \qquad \text{or} \qquad |\mu_\kappa| = \varepsilon. \tag{86}$$

We must remember, however, that the value $\mu_\kappa = 0$ must be excluded from the set admitted by equation (86) since if $\mu_\kappa = 0$ then $\eta_\kappa = \pm\infty$. Consequently, we arrive at the conclusion that the spectrum for the problem (52)–(54) consists of the real axis with the point $\mu_\kappa = 0$ excluded plus a circumference in the complex μ_κ-plane of radius ε centred at the origin

$$-\infty < \mu_\kappa < 0 \qquad \text{or} \qquad 0 < \mu_\kappa < +\infty \qquad \text{or} \qquad |\mu_\kappa| = \varepsilon. \tag{87}$$

Since the eigenvalue μ_κ is independent of the quantum number κ, in what follows we shall omit the index κ at the eigenvalue and its functions η_κ and ξ_κ.

A schematic plot of the spectrum of μ-eigenvalues is shown in figure 1. A plot of the function $\eta(\mu)$ for real μ is drawn in figure 2 while in figure 3 a plot of the function $\eta(\arg\mu)$ for μ from the circumference $|\mu| = \varepsilon$ is sketched.

The fact that η is real may be exploited to transform equations (80) and (81) to more symmetric forms. Making use of the second of the relations (18) one obtains

$$\begin{aligned} S_{\mu\kappa}(x) \xrightarrow{x\to\infty}\ & \tfrac{1}{2}D^{(+)}_{\mu\kappa}\exp[\mathrm{i}(\tfrac{1}{2}x + \eta\ln x - \tfrac{1}{2}\pi\gamma_\kappa - \sigma_{\gamma_\kappa}(\eta) - \phi^{(+)}_\kappa)] \\ & + \tfrac{1}{2}D^{(-)}_{\mu\kappa}\exp[-\mathrm{i}(\tfrac{1}{2}x + \eta\ln x - \tfrac{1}{2}\pi\gamma_\kappa - \sigma_{\gamma_\kappa}(\eta) - \phi^{(-)}_\kappa)] \end{aligned} \tag{88}$$

$$\begin{aligned} T_{\mu\kappa}(x) \xrightarrow{x\to\infty}\ & \tfrac{1}{2}\mathrm{i}\varepsilon D^{(+)}_{\mu\kappa}\exp[\mathrm{i}(\tfrac{1}{2}x + \eta\ln x - \tfrac{1}{2}\pi\gamma_\kappa - \sigma_{\gamma_\kappa}(\eta) - \phi^{(+)}_\kappa)] \\ & - \tfrac{1}{2}\mathrm{i}\varepsilon D^{(-)}_{\mu\kappa}\exp[-\mathrm{i}(\tfrac{1}{2}x + \eta\ln x - \tfrac{1}{2}\pi\gamma_\kappa - \sigma_{\gamma_\kappa}(\eta) - \phi^{(-)}_\kappa)]. \end{aligned} \tag{89}$$

Henceforth we shall find it convenient to distinguish explicitly between the Sturmians corresponding to real and complex eigenvalues. Therefore we shall make a notational change. We shall use $S^{(r)}_{\mu\kappa}(x)$ and $T^{(r)}_{\mu\kappa}(x)$ to denote the Sturmians corresponding to real eigenvalues μ and $S^{(c)}_{\mu\kappa}(x)$ and $T^{(c)}_{\mu\kappa}(x)$ to denote those Sturmians which correspond to eigenvalues from the circumference in the complex μ-plane.

In the event of real eigenvalues μ the asymptotic expressions (88) and (89) may be still simplified. Indeed, in this case the parameter ξ is real and one has

$$D_{\mu\kappa} \equiv D^{(-)}_{\mu\kappa} = D^{(+)}_{\mu\kappa} \qquad \phi_\kappa \equiv \phi^{(-)}_\kappa = \phi^{(+)}_\kappa \qquad (\mathrm{Im}\,\mu = 0). \tag{90}$$

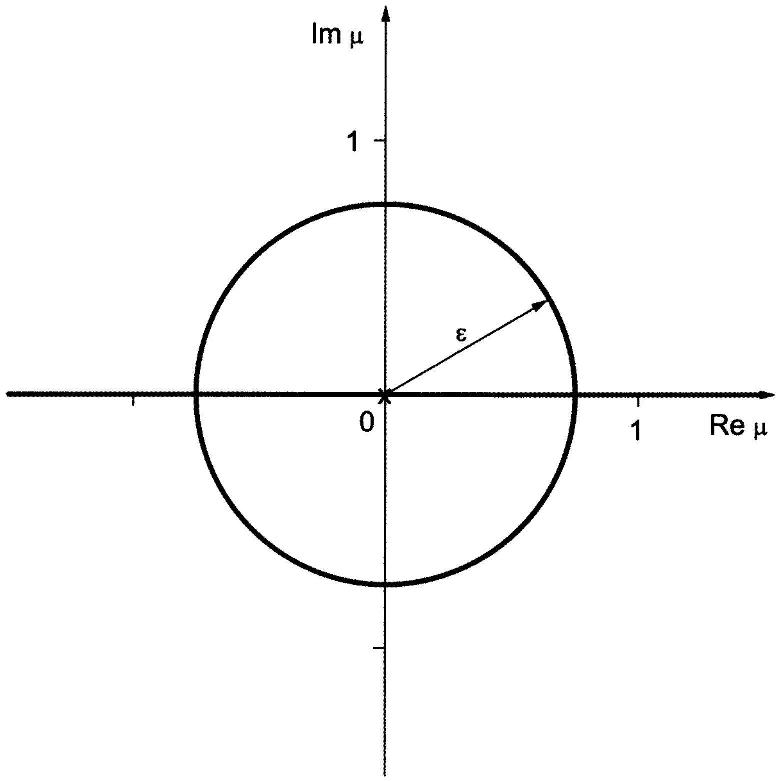

Figure 1. The spectrum of μ-eigenvalues for the Sturm–Liouville problem (52)–(54). The spectrum consists of the real axis, with zero excluded, plus the complex circumference $|\mu| = \varepsilon$.

On combining this result with equations (88) and (89) one obtains

$$S^{(r)}_{\mu_\kappa\kappa}(x) \stackrel{x\to\infty}{\longrightarrow} D_{\mu\kappa}\cos\left(\tfrac{1}{2}x + \eta\ln x - \tfrac{1}{2}\pi\gamma_\kappa - \sigma_{\gamma_\kappa}(\eta) - \phi_\kappa\right) \qquad (91)$$

$$T^{(r)}_{\mu\kappa}(x) \stackrel{x\to\infty}{\longrightarrow} -\varepsilon D_{\mu\kappa}\sin\left(\tfrac{1}{2}x + \eta\ln x - \tfrac{1}{2}\pi\gamma_\kappa - \sigma_{\gamma_\kappa}(\eta) - \phi_\kappa\right). \qquad (92)$$

It remains to investigate the problem of the orthogonality and normalization of the Sturmians $\left\{(\, S_{\mu\kappa}(x) \quad T_{\mu\kappa}(x)\,)^\top\right\}$. To this end, we consider two equations of the form (52) satisfied by the Sturmians $(\, S_{\mu\kappa}(x') \quad T_{\mu\kappa}(x'))\,)^\top$ and $(\, S_{\mu'\kappa}(x') \quad T_{\mu'\kappa}(x')\,)^\top$ corresponding to the eigenvalues μ and μ', respectively. We premultiply the equation for $(\, S_{\mu\kappa}(x') \quad T_{\mu\kappa}(x')\,)^\top$ by $(\, S_{\mu'\kappa}(x') \quad T_{\mu'\kappa}(x')\,)$, the equation for $(\, S_{\mu'\kappa}(x') \quad T_{\mu'\kappa}(x')\,)^\top$ by $(\, S_{\mu\kappa}(x') \quad T_{\mu\kappa}(x')\,)$, subtract the results, integrate from $x' = 0$ to $x' = x$ and utilize the boundary conditions at the lower integration limit obtaining

$$(\mu - \mu')\zeta\int_0^x \mathrm{d}x'\,\frac{1}{x'}[S_{\mu\kappa}(x')S_{\mu'\kappa}(x') - \mu^{-1}\mu^{'-1}T_{\mu\kappa}(x')T_{\mu'\kappa}(x')]$$
$$= S_{\mu\kappa}(x)T_{\mu'\kappa}(x) - S_{\mu'\kappa}(x)T_{\mu\kappa}(x). \qquad (93)$$

The relation (93) is valid for arbitrary $x \geqslant 0$. In particular, it holds for large values of x. Assuming in equation (93) that $x \to \infty$ and utilizing the asymptotic relations (88) and (89) one arrives at

$$\zeta\int_0^x \mathrm{d}x'\,\frac{1}{x'}[S_{\mu\kappa}(x')S_{\mu'\kappa}(x') - \mu^{-1}\mu^{'-1}T_{\mu\kappa}(x')T_{\mu'\kappa}(x')]$$

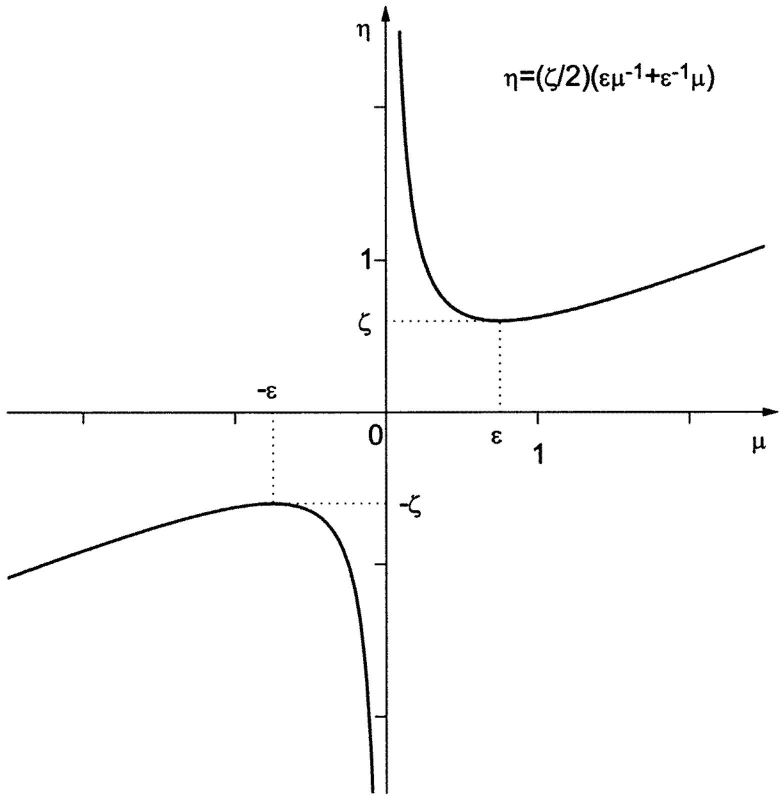

Figure 2. The plot of the function $\eta(\mu)$ defined by equation (58) for real values of μ. A positive value of ζ is assumed.

$$\begin{aligned}
&\overset{x\to\infty}{\longrightarrow} \tfrac{1}{2}\varepsilon[D^{(+)}_{\mu'\kappa}D^{(-)}_{\mu\kappa}\exp[\mathrm{i}(\phi^{(-)}_{\kappa}-\phi^{(+)'}_{\kappa})]+D^{(+)}_{\mu\kappa}D^{(-)}_{\mu'\kappa}\exp[\mathrm{i}(\phi^{(-)'}_{\kappa}-\phi^{(+)}_{\kappa})]]\\
&\times\frac{\sin[(\eta-\eta')\ln x-(\sigma_{\gamma_\kappa}(\eta)-\sigma_{\gamma_\kappa}(\eta'))]}{\mu-\mu'}\\
&+\mathrm{i}\frac{1}{2}\varepsilon\frac{D^{(+)}_{\mu'\kappa}D^{(-)}_{\mu\kappa}\exp[\mathrm{i}(\phi^{(-)}_{\kappa}-\phi^{(+)'}_{\kappa})]-D^{(+)}_{\mu\kappa}D^{(-)}_{\mu'\kappa}\exp[\mathrm{i}(\phi^{(-)'}_{\kappa}-\phi^{(+)}_{\kappa})]}{\mu-\mu'}\\
&\times\cos[(\eta-\eta')\ln x-(\sigma_{\gamma_\kappa}(\eta)-\sigma_{\gamma_\kappa}(\eta'))]. \qquad (94)
\end{aligned}$$

Initially we shall consider the case when μ is real and lies anywhere on the real axis (excluding zero) while μ' is complex and belongs to the circumference $|\mu'| = \varepsilon$. In such a case the difference $\mu - \mu'$ is certainly different from zero. Next, since μ is real, it follows from the definition (58) that $|\eta| \geqslant |\zeta|$. in contrast, since μ' is complex and $|\mu'| = \varepsilon$, one has $|\eta'| < |\zeta|$. This implies that the difference $\eta - \eta'$ premultiplying $\ln x$ on the right-hand side of equation (94) does not vanish in the case considered. When x (and consequently $\ln x$) approaches infinity, both terms on the right-hand side of equation (94) oscillate infinitely rapidly but remain bounded. Therefore, considered as an integral kernel, the right-hand side of equation (94) is effectively zero and in this sense the Sturmian functions corresponding to real and complex eigenvalues are mutually orthogonal. The relevant orthogonality relation

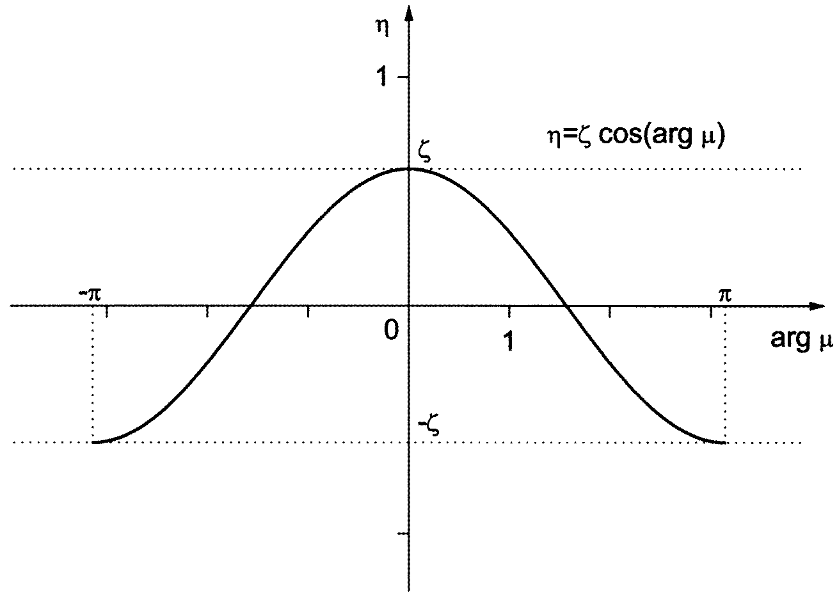

Figure 3. The plot of the function $\eta(\arg\mu)$ for complex values of μ from the circumference $|\mu| = \varepsilon$. A positive value of ζ is assumed.

is

$$\int_0^\infty \mathrm{d}x\, \frac{|Z|}{x}[S^{(r)}_{\mu\kappa}(x)S^{(c)}_{\mu'\kappa}(x) - \mu^{-1}\mu'^{-1}T^{(r)}_{\mu\kappa}(x)T^{(c)}_{\mu'\kappa}(x)] = 0. \tag{95}$$

Next consider the case when both μ and μ' are real. Rewriting the difference $\eta - \eta'$ in the form

$$\eta - \eta' = \tfrac{1}{2}\zeta(\mu - \mu')(\varepsilon^{-1} - \varepsilon\mu^{-1}\mu'^{-1}) \tag{96}$$

we find that the asymptotic limit of the fraction in the first term on the right-hand side of equation (94) is

$$\frac{\sin\left[(\eta - \eta')\ln x - (\sigma_{\gamma_\kappa}(\eta) - \sigma_{\gamma_\kappa}(\eta'))\right]}{\mu - \mu'} \xrightarrow{x\to\infty} \pi\,\mathrm{sign}[\zeta(\mu^2 - \varepsilon^2)]\delta(\mu - \mu'). \tag{97}$$

Since in the limit $x \to \infty$ the second term on the right-hand side of equation (94) oscillates infinitely rapidly but remains bounded and therefore is effectively zero, it follows that

$$\zeta\int_0^\infty \mathrm{d}x\, \frac{1}{x}\left[S^{(r)}_{\mu\kappa}(x)S^{(r)}_{\mu'\kappa}(x) - \mu^{-1}\mu'^{-1}T^{(r)}_{\mu\kappa}(x)T^{(r)}_{\mu'\kappa}(x)\right] = \pi\varepsilon D^2_{\mu\kappa}\,\mathrm{sign}[\zeta(\mu^2 - \varepsilon^2)]\,\delta(\mu - \mu') \tag{98}$$

(cf equation (90)). Imposing the normalization condition in the form

$$\int_0^\infty \mathrm{d}x\, \frac{|Z|}{x}\left[S^{(r)}_{\mu\kappa}(x)S^{(r)}_{\mu'\kappa}(x) - \mu^{-1}\mu'^{-1}T^{(r)}_{\mu\kappa}(x)T^{(r)}_{\mu'\kappa}(x)\right] = \mathrm{sign}(\mu^2 - \varepsilon^2)\,\delta(\mu - \mu') \tag{99}$$

we find the normalization factor

$$D_{\mu\kappa} = \sqrt{\frac{\alpha}{\pi\varepsilon}}. \tag{100}$$

Using this result, referring to equations (76), (77), (82) and (90) and utilizing the relations

$$\cos\phi_\kappa = \frac{1}{\sqrt{1+\left(\frac{\kappa+\gamma_\kappa}{\eta-\xi}\right)^2}} \qquad \sin\phi_\kappa = \frac{\frac{\kappa+\gamma_\kappa}{\eta-\xi}}{\sqrt{1+\left(\frac{\kappa+\gamma_\kappa}{\eta-\xi}\right)^2}} \tag{101}$$

which stem from definition (83) and from the fact that for real μ the parameter ξ is also real, we obtain the following explicit forms of the radial Sturmians normalized in the sense of equation (99)

$$S_{\mu\kappa}^{(r)}(x) = \sqrt{\frac{\alpha}{\pi\varepsilon}}\,\mathrm{e}^{(\eta-\mathrm{i}\gamma_\kappa)\pi/2}\cos\phi_\kappa\,\frac{|\Gamma(\gamma_\kappa+1+\mathrm{i}\eta)|}{\Gamma(2\gamma_\kappa+1)} \times\left[M_{-\mathrm{i}\eta,\gamma_\kappa-1/2}(\mathrm{i}x) - \mathrm{i}\frac{\eta\kappa+\xi\gamma_\kappa}{2\gamma_\kappa(2\gamma_\kappa+1)(\kappa-\gamma_\kappa)}M_{-\mathrm{i}\eta,\gamma_\kappa+1/2}(\mathrm{i}x)\right] \tag{102}$$

$$T_{\mu\kappa}^{(r)}(x) = \sqrt{\frac{\alpha\varepsilon}{\pi}}\,\mathrm{e}^{(\eta-\mathrm{i}\gamma_\kappa)\pi/2}\sin\phi_\kappa\,\frac{|\Gamma(\gamma_\kappa+1+\mathrm{i}\eta)|}{\Gamma(2\gamma_\kappa+1)} \times\left[M_{-\mathrm{i}\eta,\gamma_\kappa-1/2}(\mathrm{i}x) - \mathrm{i}\frac{\eta\kappa+\xi\gamma_\kappa}{2\gamma_\kappa(2\gamma_\kappa+1)(\kappa+\gamma_\kappa)}M_{-\mathrm{i}\eta,\gamma_\kappa+1/2}(\mathrm{i}x)\right]. \tag{103}$$

If, instead of using equations (76) and (77), we start from equations (78) and (79), we arrive at

$$S_{\mu\kappa}^{(r)}(x) = \frac{1}{2}\sqrt{\frac{\alpha}{\pi\varepsilon}}\mathrm{e}^{(\eta-\mathrm{i}\gamma_\kappa)\pi/2}\frac{|\Gamma(\gamma_\kappa+1+\mathrm{i}\eta)|}{\Gamma(2\gamma_\kappa+1)} \times(\mathrm{i}x)^{-1/2}\left[\mathrm{e}^{-\mathrm{i}\phi_\kappa}M_{-\mathrm{i}\eta-1/2,\gamma_\kappa}(\mathrm{i}x) + \mathrm{e}^{\mathrm{i}\phi_\kappa}M_{-\mathrm{i}\eta+1/2,\gamma_\kappa}(\mathrm{i}x)\right] \tag{104}$$

$$T_{\mu\kappa}^{(r)}(x) = \frac{1}{2}\mathrm{i}\sqrt{\frac{\alpha\varepsilon}{\pi}}\mathrm{e}^{(\eta-\mathrm{i}\gamma_\kappa)\pi/2}\frac{|\Gamma(\gamma_\kappa+1+\mathrm{i}\eta)|}{\Gamma(2\gamma_\kappa+1)} \times(\mathrm{i}x)^{-1/2}\left[\mathrm{e}^{-\mathrm{i}\phi_\kappa}M_{-\mathrm{i}\eta-1/2,\gamma_\kappa}(\mathrm{i}x) - \mathrm{e}^{\mathrm{i}\phi_\kappa}M_{-\mathrm{i}\eta+1/2,\gamma_\kappa}(\mathrm{i}x)\right]. \tag{105}$$

The two forms of the radial Sturmians, (102) and (103) as well as (104) and (105), are equivalent.

The functions $S_{\mu\kappa}^{(r)}(x)$ and $T_{\mu\kappa}^{(r)}(x)$ are real. This result is readily proved by utilizing the representations (104) and (105) and the complex conjugation formula (198).

Finally, we shall discuss the case when both eigenvalues μ and μ' are complex and lie on the circumference of radius ε centred at the origin. Now the situation is slightly more complicated than when both μ and μ' are real. Indeed, for complex μ and μ' we cannot normalize the Sturmians to $\delta(\mu-\mu')$ since, in principle, the Dirac delta function is not defined for complex arguments. The difficulty may be overcome, however, because the eigenvalues μ and μ' are not distributed over the whole complex plane but are confined to the circumference. Any line may be parametrized by a single real parameter and in the case discussed here it is convenient and natural to parametrize the eigenvalues μ and μ' by their arguments ψ and ψ', respectively. One has

$$\mu = \varepsilon\mathrm{e}^{\mathrm{i}\psi} \qquad -\pi < \psi \equiv \arg\mu \leqslant \pi \tag{106}$$

and similarly for μ'. With this choice of the parametrization, it follows from equations (58) and (74) that η and ξ may be also expressed in terms of ψ

$$\eta = \zeta\cos\psi \qquad \xi = \mathrm{i}\zeta\sin\psi. \tag{107}$$

The analogous relations for η' and ξ' are obtained from equation (107) replacing there η, ξ, ψ by η', ξ' and ψ', respectively. Since ψ and ψ' are real and since there are one-to-one correspondences between their values and values of μ and μ', it is possible to normalize the Sturmians to $\delta(\psi-\psi')$.

Let us consider now the fraction in the first term on the right-hand side of equation (94). In virtue of equations (106) and (107), on utilizing the relation

$$\eta-\eta'=-\zeta(\psi-\psi')\sin\left[\frac{1}{2}(\psi+\psi')\right]\left(\frac{\sin\left[\frac{1}{2}(\psi-\psi')\right]}{\frac{1}{2}(\psi-\psi')}\right) \tag{108}$$

we find the asymptotic limit of this fraction

$$\frac{\sin[(\eta-\eta')\ln x-(\sigma_{\gamma_\kappa}(\eta)-\sigma_{\gamma_\kappa}(\eta'))]}{\mu-\mu'}\xrightarrow{x\to\infty}\mathrm{i}\frac{\pi}{\varepsilon}\mathrm{e}^{-\mathrm{i}\psi}\,\mathrm{sign}(\zeta\sin\psi)\,\delta(\psi-\psi'). \tag{109}$$

Since for $x\to\infty$ the second term on the right-hand side of equation (94) is effectively zero, substitution of the result (109) to equation (94) yields

$$\begin{aligned}\zeta\int_0^\infty \mathrm{d}x\,\frac{1}{x}[S_{\mu\kappa}^{(c)}(x)S_{\mu'\kappa}^{(c)}(x)-\mu^{-1}\mu'^{-1}T_{\mu\kappa}^{(c)}(x)T_{\mu'\kappa}^{(c)}(x)]\\ =\pi D_{\mu\kappa}^{(+)}D_{\mu\kappa}^{(-)}\mathrm{e}^{\mathrm{i}(\pi/2-\psi)}\exp[\mathrm{i}(\phi_\kappa^{(-)}-\phi_\kappa^{(+)})]\,\mathrm{sign}(\zeta\sin\psi)\delta(\psi-\psi').\end{aligned} \tag{110}$$

It is then natural to impose the normalization condition in the form

$$\int_0^\infty \mathrm{d}x\,\frac{|Z|}{x}[S_{\mu\kappa}^{(c)}(x)S_{\mu'\kappa}^{(c)}(x)-\mu^{-1}\mu'^{-1}T_{\mu\kappa}^{(c)}(x)T_{\mu'\kappa}^{(c)}(x)]=\mathrm{sign}(\arg\mu)\,\delta(\arg\mu-\arg\mu') \tag{111}$$

(notice that since $-\pi<\psi\leqslant\pi$ one has $\mathrm{sign}(\sin\psi)=\mathrm{sign}\,\psi$). Comparison of equations (110) and (111) gives

$$\frac{\pi}{\alpha}D_{\mu\kappa}^{(+)}D_{\mu\kappa}^{(-)}\mathrm{e}^{\mathrm{i}(\pi/2-\psi)}\exp[\mathrm{i}(\phi_\kappa^{(-)}-\phi_\kappa^{(+)})]=1 \tag{112}$$

and upon combining this result with equation (82) one finds

$$\begin{aligned}C_{\mu\kappa}=\sqrt{\frac{\alpha}{\pi}}\exp\left[\frac{1}{2}\pi\eta+\mathrm{i}\left(\frac{1}{2}\psi-\frac{1}{2}\pi\gamma_\kappa-\frac{1}{4}\pi\right)\right]\frac{|\Gamma(\gamma_\kappa+1+\mathrm{i}\eta)|}{\Gamma(2\gamma_\kappa+1)}\\ \times\frac{\exp\left[\frac{1}{2}\mathrm{i}\left(\phi_\kappa^{(+)}-\phi_\kappa^{(-)}\right)\right]}{\sqrt{\left|1-\mathrm{i}\frac{\kappa+\gamma_\kappa}{\eta-\xi}\right|\left|1+\mathrm{i}\frac{\kappa+\gamma_\kappa}{\eta-\xi}\right|}}.\end{aligned} \tag{113}$$

It is now easy to find explicit forms of the radial Sturmians $S_{\mu\kappa}^{(c)}(x)$ and $T_{\mu\kappa}^{(c)}(x)$. From equations (76), (77) and (113) and the relation

$$\left|1\mp\mathrm{i}\frac{\kappa+\gamma_\kappa}{\eta-\xi}\right|=\sqrt{2\frac{\kappa\pm\zeta\sin\psi}{\kappa-\gamma_\kappa}} \tag{114}$$

one obtains

$$\begin{aligned}S_{\mu\kappa}^{(c)}(x)=|\zeta|\sqrt{\frac{\alpha}{2\pi}}\exp\left[\frac{1}{2}\pi\zeta\cos\psi+\mathrm{i}\left(\frac{1}{2}\psi-\frac{1}{2}\pi\gamma_\kappa-\frac{1}{4}\pi\right)\right]\exp\left[\frac{1}{2}\mathrm{i}(\phi_\kappa^{(+)}-\phi_\kappa^{(-)})\right]\\ \times\left[(\kappa+\gamma_\kappa)^2(\kappa^2-\zeta^2\sin^2\psi)\right]^{-1/4}\frac{|\Gamma(\gamma_\kappa+1+\mathrm{i}\zeta\cos\psi)|}{\Gamma(2\gamma_\kappa+1)}\\ \times\left[M_{-\mathrm{i}\zeta\cos\psi,\gamma_\kappa-1/2}(\mathrm{i}x)-\mathrm{i}\frac{\zeta(\kappa\cos\psi+\mathrm{i}\gamma_\kappa\sin\psi)}{2\gamma_\kappa(2\gamma_\kappa+1)(\kappa-\gamma_\kappa)}M_{-\mathrm{i}\zeta\cos\psi,\gamma_\kappa+1/2}(\mathrm{i}x)\right]\end{aligned} \tag{115}$$

$$T_{\mu\kappa}^{(c)}(x)=\varepsilon\zeta\,\mathrm{sign}(\kappa)\sqrt{\frac{\alpha}{2\pi}}\exp\left[\frac{1}{2}\pi\zeta\cos\psi+\mathrm{i}\left(\frac{3}{2}\psi-\frac{1}{2}\pi\gamma_\kappa-\frac{1}{4}\pi\right)\right]$$

$$\times \exp\left[\frac{1}{2}\mathrm{i}(\phi_\kappa^{(+)} - \phi_\kappa^{(-)})\right]\left[(\kappa-\gamma_\kappa)^2(\kappa^2 - \zeta^2 \sin^2\psi)\right]^{-1/4}$$
$$\times \frac{|\Gamma(\gamma_\kappa + 1 + \mathrm{i}\zeta\cos\psi)|}{\Gamma(2\gamma_\kappa+1)}\left[M_{-\mathrm{i}\zeta\cos\psi,\gamma_\kappa-1/2}(\mathrm{i}x)\right.$$
$$\left. -\mathrm{i}\frac{\zeta(\kappa\cos\psi + \mathrm{i}\gamma_\kappa\sin\psi)}{2\gamma_\kappa(2\gamma_\kappa+1)(\kappa+\gamma_\kappa)} M_{-\mathrm{i}\zeta\cos\psi,\gamma_\kappa+1/2}(\mathrm{i}x)\right]. \tag{116}$$

Equivalently, on combining equations (78), (79), (82), (83) and (113) one obtains

$$S_{\mu\kappa}^{(c)}(x) = \frac{1}{2}\sqrt{\frac{\alpha}{\pi}}\exp\left[\frac{1}{2}\pi\zeta\cos\psi + \mathrm{i}\left(\frac{1}{2}\psi - \frac{1}{2}\pi\gamma_\kappa - \frac{1}{4}\pi\right)\right]\frac{|\Gamma(\gamma_\kappa+1+\mathrm{i}\zeta\cos\psi)|}{\Gamma(2\gamma_\kappa+1)}$$
$$\times(\mathrm{i}x)^{-1/2}\left[\left(\frac{\kappa+\zeta\sin\psi}{\kappa-\zeta\sin\psi}\right)^{1/4}\exp\left[-\frac{1}{2}\mathrm{i}\left(\phi_\kappa^{(+)}+\phi_\kappa^{(-)}\right)\right]M_{-\mathrm{i}\zeta\cos\psi-1/2,\gamma_\kappa}(\mathrm{i}x)\right.$$
$$\left.+\left(\frac{\kappa-\zeta\sin\psi}{\kappa+\zeta\sin\psi}\right)^{1/4}\exp\left[\frac{1}{2}\mathrm{i}\left(\phi_\kappa^{(+)}+\phi_\kappa^{(-)}\right)\right]M_{-\mathrm{i}\zeta\cos\psi+1/2,\gamma_\kappa}(\mathrm{i}x)\right] \tag{117}$$

$$T_{\mu\kappa}^{(c)}(x) = \frac{1}{2}\varepsilon\sqrt{\frac{\alpha}{\pi}}\exp\left[\frac{1}{2}\pi\zeta\cos\psi + \mathrm{i}\left(\frac{1}{2}\psi - \frac{1}{2}\pi\gamma_\kappa + \frac{1}{4}\pi\right)\right]\frac{|\Gamma(\gamma_\kappa+1+\mathrm{i}\zeta\cos\psi)|}{\Gamma(2\gamma_\kappa+1)}$$
$$\times(\mathrm{i}x)^{-1/2}\left[\left(\frac{\kappa+\zeta\sin\psi}{\kappa-\zeta\sin\psi}\right)^{1/4}\exp\left[-\frac{1}{2}\mathrm{i}\left(\phi_\kappa^{(+)}+\phi_\kappa^{(-)}\right)\right]M_{-\mathrm{i}\zeta\cos\psi-1/2,\gamma_\kappa}(\mathrm{i}x)\right.$$
$$\left.-\left(\frac{\kappa-\zeta\sin\psi}{\kappa+\zeta\sin\psi}\right)^{1/4}\exp\left[\frac{1}{2}\mathrm{i}\left(\phi_\kappa^{(+)}+\phi_\kappa^{(-)}\right)\right]M_{-\mathrm{i}\zeta\cos\psi+1/2,\gamma_\kappa}(\mathrm{i}x)\right]. \tag{118}$$

Taking the complex conjugate of equations (117) and (118), utilizing the fact that

$$\arg\mu^* = -\arg\mu \qquad \phi_\kappa^{(\pm)}(\mu^*) = \phi_\kappa^{(\mp)}(\mu) \tag{119}$$

and applying formula (198) we find that the functions $S_{\mu\kappa}^{(c)}(x)$ and $T_{\mu\kappa}^{(c)}(x)$ possess the symmetry property

$$[S_{\mu\kappa}^{(c)}(x)]^* = \mathrm{i}S_{\mu^*\kappa}^{(c)}(x) \qquad [T_{\mu\kappa}^{(c)}(x)]^* = \mathrm{i}T_{\mu^*\kappa}^{(c)}(x). \tag{120}$$

Making use of the orthogonality relations (95), (99) and (111) it is possible to predict the form of a closure relation obeyed by the radial Sturmians. After little thought one finds

$$\frac{|Z|}{x'}\wp\int_{-\infty}^{\infty}\mathrm{d}\mu\ \mathrm{sign}(\mu^2-\varepsilon^2)\begin{pmatrix} S_{\mu\kappa}^{(r)}(x) \\ \mu^{-1}T_{\mu\kappa}^{(r)}(x)\end{pmatrix}\begin{pmatrix} S_{\mu\kappa}^{(r)}(x') & -\mu^{-1}T_{\mu\kappa}^{(r)}(x')\end{pmatrix}$$
$$+\frac{|Z|}{x'}\int_{-\pi}^{\pi}\mathrm{d}(\arg\mu)\ \mathrm{sign}(\arg\mu)\begin{pmatrix} S_{\mu\kappa}^{(c)}(x) \\ \mu^{-1}T_{\mu\kappa}^{(c)}(x)\end{pmatrix}\begin{pmatrix} S_{\mu\kappa}^{(c)}(x') & -\mu^{-1}T_{\mu\kappa}^{(c)}(x')\end{pmatrix}$$
$$= \delta(x-x')I \tag{121}$$

where $\wp$ denotes the principal value of the integral following this symbol. It must be distinctly stated here that although there is a good deal to believe that the closure relation (121) holds, it appears here as a postulate rather than as a sound theorem. Unfortunately, the method which we used in [4] to prove the analogous closure relation for the discrete Dirac–Coulomb Sturmians cannot be applied in the case discussed in this paper. We have not been able to find a rigorous proof and therefore the problem of showing the validity of the relation (121) is left open.

With the radial Sturmians found above we may construct the three-dimensional four-component spinor Sturmians

$$\Phi^{(r,c)}_{\mu\kappa m_j}(E,\boldsymbol{r}) = \frac{1}{r}\begin{pmatrix} S^{(r,c)}_{\mu\kappa}(2\lambda r)\Omega_{\kappa m_j}(\boldsymbol{n}) \\ \mathrm{i}T^{(r,c)}_{\mu\kappa}(2\lambda r)\Omega_{-\kappa m_j}(\boldsymbol{n}) \end{pmatrix}. \tag{122}$$

The orthogonality relations satisfied by the functions (122), the analogues of the relations (99), (111) and (95), are

$$\int_{\mathcal{R}^3} \mathrm{d}^3\boldsymbol{r}\, \frac{|Z|}{r} \Phi^{(r)\dagger}_{\mu\kappa m_j}(E,\boldsymbol{r})\mathcal{V}_\mu \beta \mathcal{V}_{\mu'} \Phi^{(r)}_{\mu'\kappa' m_j'}(E,\boldsymbol{r}) = \mathrm{sign}(\mu^2-\varepsilon^2)\delta(\mu-\mu')\delta_{\kappa\kappa'}\delta_{m_j m_j'} \tag{123}$$

$$\int_{\mathcal{R}^3} \mathrm{d}^3\boldsymbol{r}\, \frac{|Z|}{r} \Phi^{(c)\dagger}_{\mu^*\kappa m_j}(E,\boldsymbol{r})\mathcal{V}^\dagger_{\mu^*} \beta \mathcal{V}_{\mu'} \Phi^{(c)}_{\mu'\kappa' m_j'}(E,\boldsymbol{r}) = \mathrm{i}\,\mathrm{sign}(\arg\mu)\delta(\arg\mu-\arg\mu')\delta_{\kappa\kappa'}\delta_{m_j m_j'} \tag{124}$$

and

$$\int_{\mathcal{R}^3} \mathrm{d}^3\boldsymbol{r}\, \frac{|Z|}{r} \Phi^{(c)\dagger}_{\mu^*\kappa m_j}(E,\boldsymbol{r})\mathcal{V}^\dagger_{\mu^*} \beta \mathcal{V}_{\mu'} \Phi^{(r)}_{\mu'\kappa' m_j'}(E,\boldsymbol{r}) = 0 \tag{125}$$

$$\int_{\mathcal{R}^3} \mathrm{d}^3\boldsymbol{r}\, \frac{|Z|}{r} \Phi^{(r)\dagger}_{\mu\kappa m_j}(E,\boldsymbol{r})\mathcal{V}_\mu \beta \mathcal{V}_{\mu'} \Phi^{(c)}_{\mu'\kappa' m_j'}(E,\boldsymbol{r}) = 0 \tag{126}$$

respectively, where

$$\mathcal{V}_\mu = \begin{pmatrix} I & 0 \\ 0 & \mu^{-1}I \end{pmatrix}. \tag{127}$$

Throughout the dagger denotes the matrix Hermitian conjugation. The three-dimensional analogue of the closure relation (121) (cf the remark following the latter equation) is

$$\begin{aligned}\frac{|Z|}{r'}\sum_{\kappa m_j} \wp \int_{-\infty}^{\infty} \mathrm{d}\mu\, \mathrm{sign}(\mu^2-\varepsilon^2)\mathcal{V}_\mu \Phi^{(r)}_{\mu\kappa m_j}(E,\boldsymbol{r})\Phi^{(r)\dagger}_{\mu\kappa m_j}(E,\boldsymbol{r}')\mathcal{V}_\mu\beta \\ -\mathrm{i}\frac{|Z|}{r'}\sum_{\kappa m_j}\int_{-\pi}^{\pi} \mathrm{d}(\arg\mu)\,\mathrm{sign}(\arg\mu)\mathcal{V}_\mu \Phi^{(c)}_{\mu\kappa m_j}(E,\boldsymbol{r})\Phi^{(c)\dagger}_{\mu^*\kappa m_j}(E,\boldsymbol{r}')\mathcal{V}^\dagger_{\mu^*}\beta \\ = \delta(\boldsymbol{r}-\boldsymbol{r}')\,\mathcal{I}.\end{aligned} \tag{128}$$

5. The continuum Dirac–Coulomb Sturmian functions of the second kind

Besides the Sturmians discussed in the preceding section there exists another set of Sturmian functions related to the continuum Dirac–Coulomb problem. The continuum Dirac–Coulomb Sturmian functions of the second kind,

$$\overline{\Phi}_{\bar{\mu}_\kappa\kappa m_j}(E,\boldsymbol{r}) = \frac{1}{r}\begin{pmatrix} \overline{S}_{\bar{\mu}_\kappa\kappa}(2\lambda r)\Omega_{\kappa m_j}(\boldsymbol{n}) \\ \mathrm{i}\overline{T}_{\bar{\mu}_\kappa\kappa}(2\lambda r)\Omega_{-\kappa m_j}(\boldsymbol{n}) \end{pmatrix} \tag{129}$$

(here λ has the same meaning as in section 4), are defined as those simultaneous eigenfunctions of the operators $\mathcal{K}$ and J_z (cf equation (39)) which are solutions of the Dirac equation

$$\left[-\mathrm{i}c\hbar\boldsymbol{\alpha}\cdot\boldsymbol{\nabla} + \overline{\mathcal{M}}_\kappa(\beta mc^2 - E\mathcal{I}) - \frac{Ze^2}{r}\right]\overline{\Phi}_{\bar{\mu}_\kappa\kappa m_j}(E,\boldsymbol{r}) = 0 \tag{130}$$

and near the singular points $r=0$ and $r=\infty$ behave as

$$r\overline{\Phi}_{\bar{\mu}_\kappa\kappa m_j}(E,\boldsymbol{r}) \overset{l}{\sim} r \to 0 r^{\gamma_\kappa} \qquad r\overline{\Phi}_{\bar{\mu}_\kappa\kappa m_j}(E,\boldsymbol{r}) \text{ bounded for } r\to\infty. \tag{131}$$

In equation (130) $\overline{\mathcal{M}}_\kappa$ is a matrix of the form

$$\overline{\mathcal{M}}_\kappa = \begin{pmatrix} \bar{\mu}_\kappa I & 0 \\ 0 & \bar{\mu}_\kappa^{-1} I \end{pmatrix} \tag{132}$$

and $\bar{\mu}_\kappa$ is an eigenvalue for the problem. Separating off the angular part of the problem and changing the independent variable from r to $x = 2\lambda r$, we find that the radial Sturmians of the second kind obey the Sturm–Liouville problem consisting of a coupled set of differential equations

$$\begin{pmatrix} -\bar{\mu}_\kappa \varepsilon/2 - \zeta/x & -\mathrm{d}/\mathrm{d}x + \kappa/x \\ \mathrm{d}/\mathrm{d}x + \kappa/x & -\bar{\mu}_\kappa^{-1}\varepsilon^{-1}/2 - \zeta/x \end{pmatrix} \begin{pmatrix} \overline{S}_{\bar{\mu}_\kappa \kappa}(x) \\ \overline{T}_{\bar{\mu}_\kappa \kappa}(x) \end{pmatrix} = 0 \qquad (0 \leqslant x < \infty) \tag{133}$$

and boundary conditions

$$\overline{S}_{\bar{\mu}_\kappa \kappa}(x) \overset{x\to 0}{\sim} x^{\gamma_\kappa} \qquad \overline{T}_{\bar{\mu}_\kappa \kappa}(x) \overset{x\to 0}{\sim} x^{\gamma_\kappa} \tag{134}$$

$$\overline{S}_{\bar{\mu}_\kappa \kappa}(x) \text{ and } \overline{T}_{\bar{\mu}_\kappa \kappa}(x) \text{ bounded for } x \to \infty. \tag{135}$$

The problem (133)–(135) need not be solved directly. Indeed, a comparison of the structures of the two problems (52)–(54) and (133)–(135) shows that the eigenvalue $\bar{\mu}_\kappa$ and the eigenfunctions $\overline{S}_{\bar{\mu}_\kappa \kappa}(x)$ and $\overline{T}_{\bar{\mu}_\kappa \kappa}(x)$ are related to the solutions of the problem (52)–(54) in the following manner

$$\bar{\mu}_\kappa = \mu_\kappa^{-1} \tag{136}$$

(this implies that the spectrum of $\bar{\mu}_\kappa$-eigenvalues consists of the real axis with zero excluded plus a circumference in the complex $\bar{\mu}_\kappa$-plane of radius ε^{-1} centred at the origin) and

$$\overline{S}_{\bar{\mu}_\kappa \kappa}(x) = \text{constant} \times S_{\mu_\kappa \kappa}(x) \qquad \overline{T}_{\bar{\mu}_\kappa \kappa}(x) = \text{constant} \times \mu_\kappa^{-1} T_{\mu_\kappa \kappa}(x). \tag{137}$$

This may be verified by direct substitution. Henceforth we shall choose the constant in equation (137) equal to unity. Omitting the unnecessary index at the eigenvalue (cf the remark following equation (87)) we have

$$\overline{S}_{\bar{\mu}\kappa}(x) = S_{\mu\kappa}(x) \qquad \overline{T}_{\bar{\mu}\kappa}(x) = \mu^{-1} T_{\mu\kappa}(x) \tag{138}$$

and, consequently,

$$\overline{\Phi}_{\bar{\mu}\kappa m_j}(E, \boldsymbol{r}) = \mathcal{V}_\mu \Phi_{\mu\kappa m_j}(E, \boldsymbol{r}). \tag{139}$$

The matrix $\mathcal{V}_\mu$ has been defined by equation (127).

The results (136) and (138) and the relations

$$\begin{cases} \delta(\mu - \mu') = \bar{\mu}^2 \delta(\bar{\mu} - \bar{\mu}') & (\mu,\ \mu' \text{ real}) \\ \arg\mu = -\arg\bar{\mu} & (\mu \text{ complex}) \end{cases} \tag{140}$$

allow us to deduce from equations (99), (111), (95) and (121) the following orthogonality and closure relations satisfied by the radial Sturmians $\{\overline{S}_{\bar{\mu}\kappa}(x)\}$ and $\{\overline{T}_{\bar{\mu}\kappa}(x)\}$

$$\int_0^\infty \mathrm{d}x\, \frac{|Z|}{x} [\overline{S}^{(r)}_{\bar{\mu}\kappa}(x)\overline{S}^{(r)}_{\bar{\mu}'\kappa}(x) - \overline{T}^{(r)}_{\bar{\mu}\kappa}(x)\overline{T}^{(r)}_{\bar{\mu}'\kappa}(x)] = \bar{\mu}^2\, \mathrm{sign}(1 - \varepsilon^2\bar{\mu}^2)\delta(\bar{\mu} - \bar{\mu}') \tag{141}$$

$$\int_0^\infty \mathrm{d}x\, \frac{|Z|}{x} [\overline{S}^{(c)}_{\bar{\mu}\kappa}(x)\overline{S}^{(c)}_{\bar{\mu}'\kappa}(x) - \overline{T}^{(c)}_{\bar{\mu}\kappa}(x)\overline{T}^{(c)}_{\bar{\mu}'\kappa}(x)] = -\,\mathrm{sign}(\arg\bar{\mu})\delta(\arg\bar{\mu} - \arg\bar{\mu}') \tag{142}$$

$$\int_0^\infty \mathrm{d}x\, \frac{|Z|}{x} [\overline{S}^{(r)}_{\bar{\mu}\kappa}(x)\overline{S}^{(c)}_{\bar{\mu}'\kappa}(x) - \overline{T}^{(r)}_{\bar{\mu}\kappa}(x)\overline{T}^{(c)}_{\bar{\mu}'\kappa}(x)] = 0 \tag{143}$$

and

$$\frac{|Z|}{x'}\wp\int_{-\infty}^{\infty}\mathrm{d}\bar{\mu}\,\bar{\mu}^{-2}\,\mathrm{sign}(1-\varepsilon^2\bar{\mu}^2)\begin{pmatrix}\overline{S}^{(r)}_{\bar{\mu}\kappa}(x)\\ \overline{T}^{(r)}_{\bar{\mu}\kappa}(x)\end{pmatrix}(\,\overline{S}^{(r)}_{\bar{\mu}\kappa}(x') \quad -\overline{T}^{(r)}_{\bar{\mu}\kappa}(x')\,)$$
$$-\frac{|Z|}{x'}\int_{-\pi}^{\pi}\mathrm{d}(\arg\bar{\mu})\,\mathrm{sign}(\arg\bar{\mu})\begin{pmatrix}\overline{S}^{(c)}_{\bar{\mu}\kappa}(x)\\ \overline{T}^{(c)}_{\bar{\mu}\kappa}(x)\end{pmatrix}(\,\overline{S}^{(c)}_{\bar{\mu}\kappa}(x') \quad -\overline{T}^{(c)}_{\bar{\mu}\kappa}(x')\,)$$
$$=\delta(x-x')\,I. \tag{144}$$

Similarly, from equations (136), (139), (123)–(126) and (128) one infers the following orthogonality and closure relations for the three-dimensional Sturmians $\{\overline{\Phi}_{\bar{\mu}\kappa m_j}(E,\boldsymbol{r})\}$

$$\int_{\mathcal{R}^3}\mathrm{d}^3\boldsymbol{r}\,\frac{|Z|}{r}\overline{\Phi}^{(r)\dagger}_{\bar{\mu}\kappa m_j}(E,\boldsymbol{r})\beta\overline{\Phi}^{(r)}_{\bar{\mu}'\kappa' m_j'}(E,\boldsymbol{r})=\bar{\mu}^2\,\mathrm{sign}(1-\varepsilon^2\bar{\mu}^2)\delta(\bar{\mu}-\bar{\mu}')\delta_{\kappa\kappa'}\delta_{m_j m_j'} \tag{145}$$

$$\int_{\mathcal{R}^3}\mathrm{d}^3\boldsymbol{r}\,\frac{|Z|}{r}\overline{\Phi}^{(c)\dagger}_{\bar{\mu}^*\kappa m_j}(E,\boldsymbol{r})\beta\overline{\Phi}^{(c)}_{\bar{\mu}'\kappa' m_j'}(E,\boldsymbol{r})=-\mathrm{i}\,\mathrm{sign}(\arg\bar{\mu})\delta(\arg\bar{\mu}-\arg\bar{\mu}')\delta_{\kappa\kappa'}\delta_{m_j m_j'} \tag{146}$$

$$\int_{\mathcal{R}^3}\mathrm{d}^3\boldsymbol{r}\,\frac{|Z|}{r}\overline{\Phi}^{(c)\dagger}_{\bar{\mu}^*\kappa m_j}(E,\boldsymbol{r})\beta\overline{\Phi}^{(r)}_{\bar{\mu}'\kappa' m_j'}(E,\boldsymbol{r})=0 \tag{147}$$

$$\int_{\mathcal{R}^3}\mathrm{d}^3\boldsymbol{r}\,\frac{|Z|}{r}\overline{\Phi}^{(r)\dagger}_{\bar{\mu}\kappa m_j}(E,\boldsymbol{r})\beta\overline{\Phi}^{(c)}_{\bar{\mu}'\kappa' m_j'}(E,\boldsymbol{r})=0 \tag{148}$$

and

$$\frac{|Z|}{r'}\sum_{\kappa m_j}\wp\int_{-\infty}^{\infty}\mathrm{d}\bar{\mu}\,\bar{\mu}^{-2}\,\mathrm{sign}(1-\varepsilon^2\bar{\mu}^2)\overline{\Phi}^{(r)}_{\bar{\mu}\kappa m_j}(E,\boldsymbol{r})\overline{\Phi}^{(r)\dagger}_{\bar{\mu}\kappa m_j}(E,\boldsymbol{r}')\beta$$
$$+\mathrm{i}\frac{|Z|}{r'}\sum_{\kappa m_j}\int_{-\pi}^{\pi}\mathrm{d}(\arg\bar{\mu})\,\mathrm{sign}(\arg\bar{\mu})\overline{\Phi}^{(c)}_{\bar{\mu}\kappa m_j}(E,\boldsymbol{r})\overline{\Phi}^{(c)\dagger}_{\bar{\mu}^*\kappa m_j}(E,\boldsymbol{r}')\beta$$
$$=\delta(\boldsymbol{r}-\boldsymbol{r}')\,\mathcal{I}. \tag{149}$$

The reader has certainly noticed that in obtaining the orthogonality and closure relations for the Sturmians $\{\Phi_{\mu\kappa m_j}(E,\boldsymbol{r})\}$ and $\{(\,S_{\mu\kappa}(x) \quad T_{\mu\kappa}(x)\,)^{\top}\}$ discussed in section 4 we have exploited the form and the properties of the differential equations obeyed by these functions. In contrast, in deriving such relations for the Sturmians of the second kind we have simply transformed equations (95), (99), (111), (121), (123)–(126) and (128) without any reference to the differential equations satisfied by the functions $\{\overline{\Phi}_{\bar{\mu}\kappa m_j}(E,\boldsymbol{r})\}$ and $\{(\,\overline{S}_{\bar{\mu}\kappa}(x) \quad \overline{T}_{\bar{\mu}\kappa}(x)\,)^{\top}\}$. This suggests that (presumably) distinct orthogonality and closure relations for the Sturmians of the second kind (and, as a consequence of the relations (138) and (139), for the Sturmians of the first kind found in section 4, too) might be found by exploiting properties of the differential equations (130) and (133). This is indeed the case and initially we shall find the second set of orthogonality relations for the radial Sturmians of the second kind $\{(\,cc\overline{S}_{\bar{\mu}\kappa}(x) \quad \overline{T}_{\bar{\mu}\kappa}(x)\,)^{\top}\}$. To this end we consider two differential equations of the form (133) satisfied by the functions $(\,cc\overline{S}_{\bar{\mu}\kappa}(x') \quad \overline{T}_{\bar{\mu}\kappa}(x')\,)^{\top}$ and $(\,cc\overline{S}_{\bar{\mu}'\kappa}(x') \quad \overline{T}_{\bar{\mu}'\kappa}(x')\,)^{\top}$, respectively. We premultiply the equation for $(\,cc\overline{S}_{\bar{\mu}\kappa}(x') \quad \overline{T}_{\bar{\mu}\kappa}(x')\,)^{\top}$ by $(\,cc\overline{S}_{\bar{\mu}'\kappa}(x') \quad \overline{T}_{\bar{\mu}'\kappa}(x')\,)$, the equation for $(\,cc\overline{S}_{\overline{\mu}'\kappa}(x') \quad \overline{T}_{\bar{\mu}'\kappa}(x')\,)^{\top}$ by $(\,cc\overline{S}_{\bar{\mu}\kappa}(x') \quad \overline{T}_{\bar{\mu}\kappa}(x')\,)$, subtract the results and integrate from $x'=0$ to $x'=x$. Using the fact that the radial Sturmians vanish at the lower integration limit, we obtain

$$\tfrac{1}{2}(\bar{\mu}-\bar{\mu}')\int_0^x\mathrm{d}x'\,[\varepsilon\overline{S}_{\bar{\mu}\kappa}(x')\overline{S}_{\bar{\mu}'\kappa}(x')-\bar{\mu}^{-1}\bar{\mu}^{'-1}\varepsilon^{-1}\overline{T}_{\bar{\mu}\kappa}(x')\overline{T}_{\bar{\mu}'\kappa}(x')]$$
$$=\overline{S}_{\bar{\mu}\kappa}(x)\overline{T}_{\bar{\mu}'\kappa}(x)-\overline{S}_{\bar{\mu}'\kappa}(x)\overline{T}_{\bar{\mu}\kappa}(x). \tag{150}$$

If x is sufficiently large, the Sturmians appearing on the right-hand side of equation (150) may be replaced by their asymptotic forms which are readily derivable from equations (88), (89) and (138). After somewhat tedious manipulations one finds

$$\begin{aligned}\int_0^x \mathrm{d}x' \, [\varepsilon \overline{S}_{\bar{\mu}\kappa}(x')\overline{S}_{\bar{\mu}'\kappa}(x') - \bar{\mu}^{-1}\bar{\mu}'^{-1}\varepsilon^{-1}\overline{T}_{\bar{\mu}\kappa}(x')\overline{T}_{\bar{\mu}'\kappa}(x')] \stackrel{x\to\infty}{\longrightarrow} \tfrac{1}{2}\varepsilon(\bar{\mu}+\bar{\mu}')[D^{(+)}_{\mu'\kappa}D^{(-)}_{\mu\kappa} \\ \times \exp[\mathrm{i}(\phi^{(-)}_\kappa - \phi^{(+)'}_\kappa)] + D^{(+)}_{\mu\kappa}D^{(-)}_{\mu'\kappa}\exp[\mathrm{i}(\phi^{(-)'}_\kappa - \phi^{(+)}_\kappa)]] \\ \times \frac{\sin[(\eta-\eta')\ln x - (\sigma_{\gamma_\kappa}(\eta) - \sigma_{\gamma_\kappa}(\eta'))]}{\bar{\mu}-\bar{\mu}'} + \mathrm{i}\frac{1}{2}\varepsilon(\bar{\mu}+\bar{\mu}') \\ \frac{[D^{(+)}_{\mu'\kappa}D^{(-)}_{\mu\kappa}\exp[\mathrm{i}(\phi^{(-)}_\kappa - \phi^{(+)'}_\kappa)] - D^{(+)}_{\mu\kappa}D^{(-)}_{\mu'\kappa}\exp[\mathrm{i}(\phi^{(-)'}_\kappa - \phi^{(+)}_\kappa)]]}{\bar{\mu}-\bar{\mu}'} \\ \times \cos[(\eta-\eta')\ln x - (\sigma_{\gamma_\kappa}(\eta) - \sigma_{\gamma_\kappa}(\eta'))] \\ + \tfrac{1}{2}\varepsilon[D^{(+)}_{\mu\kappa}D^{(+)}_{\mu'\kappa}\exp[-\mathrm{i}(\phi^{(+)}_\kappa + \phi^{(+)'}_\kappa)] + D^{(-)}_{\mu\kappa}D^{(-)}_{\mu'\kappa}\exp[\mathrm{i}(\phi^{(-)}_\kappa + \phi^{(-)'}_\kappa)]] \\ \times \sin[x + (\eta+\eta')\ln x - \pi\gamma_\kappa - (\sigma_{\gamma_\kappa}(\eta) + \sigma_{\gamma_\kappa}(\eta'))] \\ - \mathrm{i}\tfrac{1}{2}\varepsilon[D^{(+)}_{\mu\kappa}D^{(+)}_{\mu'\kappa}\exp[-\mathrm{i}(\phi^{(+)}_\kappa + \phi^{(+)'}_\kappa)] - D^{(-)}_{\mu\kappa}D^{(-)}_{\mu'\kappa}\exp[\mathrm{i}(\phi^{(-)}_\kappa + \phi^{(-)'}_\kappa)]] \\ \times \cos[x + (\eta+\eta')\ln x - \pi\gamma_\kappa - (\sigma_{\gamma_\kappa}(\eta) + \sigma_{\gamma_\kappa}(\eta'))]. \end{aligned} \tag{151}$$

In the limit $x \to \infty$ all terms on the right-hand side of equation (151) oscillate infinitely rapidly but the first one becomes singular for $\bar{\mu} = \bar{\mu}'$ (this corresponds to $\mu = \mu'$) while the second, third and fourth terms are always bounded. The argument similar to that following equation (94) leads to the conclusion that in the limit $x \to \infty$ the second, third and fourth terms are effectively zero. Therefore one has

$$\begin{aligned}\int_0^x \mathrm{d}x' \, [\varepsilon \overline{S}_{\bar{\mu}\kappa}(x')\overline{S}_{\bar{\mu}'\kappa}(x') - \bar{\mu}^{-1}\bar{\mu}'^{-1}\varepsilon^{-1}\overline{T}_{\bar{\mu}\kappa}(x')\overline{T}_{\bar{\mu}'\kappa}(x')] \stackrel{x\to\infty}{\longrightarrow} \tfrac{1}{2}\varepsilon(\bar{\mu}+\bar{\mu}')[D^{(+)}_{\mu'\kappa}D^{(-)}_{\mu\kappa} \\ \times \exp[\mathrm{i}(\phi^{(-)}_\kappa - \phi^{(+)'}_\kappa)] + D^{(+)}_{\mu\kappa}D^{(-)}_{\mu'\kappa}\exp[\mathrm{i}(\phi^{(-)'}_\kappa - \phi^{(+)}_\kappa)]] \\ \times \frac{\sin[(\eta-\eta')\ln x - (\sigma_{\gamma_\kappa}(\eta) - \sigma_{\gamma_\kappa}(\eta'))]}{\bar{\mu}-\bar{\mu}'}\end{aligned} \tag{152}$$

and it remains to analyse the term on the right-hand side of equation (152).

The simplest case occurs when $\bar{\mu}$ is real and $\bar{\mu}'$ is complex. An analysis identical to the one preceding equation (95) shows that in this case the radial Sturmians of the second kind are orthogonal in the sense of

$$\int_0^\infty \mathrm{d}x [\overline{S}^{(r)}_{\bar{\mu}\kappa}(x)\overline{S}^{(c)}_{\bar{\mu}'\kappa}(x) - \bar{\mu}^{-1}\bar{\mu}'^{-1}\varepsilon^{-2}\overline{T}^{(r)}_{\bar{\mu}\kappa}(x)\overline{T}^{(c)}_{\bar{\mu}'\kappa}(x)] = 0. \tag{153}$$

The cases when $\bar{\mu}$ and $\bar{\mu}'$ are either both real or both complex are more involved. Consider at first the case when $\bar{\mu}$ and $\bar{\mu}'$ are real. Then one has (cf the definition (58))

$$\eta - \eta' = \tfrac{1}{2}\zeta(\bar{\mu}-\bar{\mu}')(\varepsilon - \varepsilon^{-1}\bar{\mu}^{-1}\bar{\mu}'^{-1}) \tag{154}$$

and in the limit $x \to \infty$

$$\frac{\sin[(\eta-\eta')\ln x - (\sigma_{\gamma_\kappa}(\eta) - \sigma_{\gamma_\kappa}(\eta'))]}{\bar{\mu}-\bar{\mu}'} \stackrel{x\to\infty}{\longrightarrow} -\pi \, \mathrm{sign}[\zeta(1-\varepsilon^2\bar{\mu}^2)]\delta(\bar{\mu}-\bar{\mu}'). \tag{155}$$

On combining this result with equations (90), (100) and (152) we arrive at the orthogonality relation

$$\begin{aligned}\int_0^\infty \mathrm{d}x \, [\overline{S}^{(r)}_{\bar{\mu}\kappa}(x)\overline{S}^{(r)}_{\bar{\mu}'\kappa}(x) - \bar{\mu}^{-1}\bar{\mu}'^{-1}\varepsilon^{-2}\overline{T}^{(r)}_{\bar{\mu}\kappa}(x)\overline{T}^{(r)}_{\bar{\mu}'\kappa}(x)] \\ = -2\alpha\varepsilon^{-1}\bar{\mu}\,\mathrm{sign}[\zeta(1-\varepsilon^2\bar{\mu}^2)]\delta(\bar{\mu}-\bar{\mu}').\end{aligned} \tag{156}$$

Consider now the case when both $\bar{\mu}$ and $\bar{\mu}'$ are complex and belong to the circumference $|\bar{\mu}| = |\bar{\mu}'| = \varepsilon^{-1}$. Then one has

$$\eta = \zeta \cos\overline{\psi} \qquad \xi = -\mathrm{i}\zeta \sin\overline{\psi} \qquad (-\pi \leqslant \overline{\psi} \equiv \arg\bar{\mu} < \pi) \tag{157}$$

and, consequently,

$$\eta - \eta' = -\zeta(\overline{\psi} - \overline{\psi}') \sin[\tfrac{1}{2}(\overline{\psi} + \overline{\psi}')] \left(\frac{\sin[\frac{1}{2}(\overline{\psi} - \overline{\psi}')]}{\frac{1}{2}(\overline{\psi} - \overline{\psi}')} \right). \tag{158}$$

Hence, it follows that

$$\frac{\sin\left[(\eta - \eta')\ln x - (\sigma_{\gamma_\kappa}(\eta) - \sigma_{\gamma_\kappa}(\eta'))\right]}{\bar{\mu} - \bar{\mu}'} \xrightarrow{x\to\infty} \mathrm{i}\pi\varepsilon \mathrm{e}^{-\mathrm{i}\overline{\psi}} \,\mathrm{sign}(\zeta \sin\overline{\psi})\delta(\overline{\psi} - \overline{\psi}') \tag{159}$$

and combining this result with equations (112) and (152) yields the orthogonality relation

$$\int_0^\infty \mathrm{d}x\, [\overline{S}^{(c)}_{\bar{\mu}\kappa}(x)\overline{S}^{(c)}_{\bar{\mu}'\kappa}(x) - \bar{\mu}^{-1}\bar{\mu}'^{-1}\varepsilon^{-2}\overline{T}^{(c)}_{\bar{\mu}\kappa}(x)\overline{T}^{(c)}_{\bar{\mu}'\kappa}(x)]$$
$$= 2\alpha\varepsilon^{-1}\bar{\mu}^{-1}\,\mathrm{sign}(\zeta \arg\bar{\mu})\delta(\arg\bar{\mu} - \arg\bar{\mu}'). \tag{160}$$

Note that relations (153), (156) and (160) differ from the relations (143), (141) and (142) obtained before.

From the relations (153), (156) and (160) we may predict the form of the *second* (i.e. different from that given by equation (144)) closure relation obeyed by the radial Sturmians $\{\overline{S}_{\bar{\mu}\kappa}(x)\}$ and $\{\overline{T}_{\bar{\mu}\kappa}(x)\}$. We find

$$-\frac{\varepsilon}{2\alpha}\wp\int_{-\infty}^{\infty} \mathrm{d}\bar{\mu}\bar{\mu}^{-1}\,\mathrm{sign}[\zeta(1 - \varepsilon^2\bar{\mu}^2)] \begin{pmatrix} \overline{S}^{(r)}_{\bar{\mu}\kappa}(x) \\ \bar{\mu}^{-1}\overline{T}^{(r)}_{\bar{\mu}\kappa}(x) \end{pmatrix} (\,\overline{S}^{(r)}_{\bar{\mu}\kappa}(x') \quad -\bar{\mu}^{-1}\varepsilon^{-2}\overline{T}^{(r)}_{\bar{\mu}\kappa}(x')\,)$$
$$+\frac{\varepsilon}{2\alpha}\int_{-\pi}^{\pi} \mathrm{d}(\arg\bar{\mu})\,\bar{\mu}\,\mathrm{sign}(\zeta \arg\bar{\mu}) \begin{pmatrix} \overline{S}^{(c)}_{\bar{\mu}\kappa}(x) \\ \bar{\mu}^{-1}\overline{T}^{(c)}_{\bar{\mu}\kappa}(x) \end{pmatrix}$$
$$\times (\,\overline{S}^{(c)}_{\bar{\mu}\kappa}(x') \quad -\bar{\mu}^{-1}\varepsilon^{-2}\overline{T}^{(c)}_{\bar{\mu}\kappa}(x')\,)$$
$$= \delta(x - x')I. \tag{161}$$

The remarks following equation (121) also apply here.

The orthogonality and closure relations for the three-dimensional Sturmians of the second kind $\{\overline{\Phi}_{\bar{\mu}\kappa m_j}(E, \boldsymbol{r})\}$, analogous to the results (156), (160), (153) and (161), respectively, are

$$\int_{\mathcal{R}^3} \mathrm{d}^3\boldsymbol{r}\, \overline{\Phi}^{(r)\dagger}_{\bar{\mu}\kappa m_j}(E, \boldsymbol{r})\overline{\mathcal{V}}_{\bar{\mu}}(mc^2\mathcal{I} - \beta E)\overline{\mathcal{V}}_{\bar{\mu}'}\overline{\Phi}^{(r)}_{\bar{\mu}'\kappa' m_j'}(E, \boldsymbol{r})$$
$$= c\overline{h}\alpha\bar{\mu}\,\mathrm{sign}[\zeta E(1 - \varepsilon^2\bar{\mu}^2)]\delta(\bar{\mu} - \bar{\mu}')\delta_{\kappa\kappa'}\delta_{m_j m_j'} \tag{162}$$

$$\int_{\mathcal{R}^3} \mathrm{d}^3\boldsymbol{r}\, \overline{\Phi}^{(c)\dagger}_{\bar{\mu}^*\kappa m_j}(E, \boldsymbol{r})\overline{\mathcal{V}}^\dagger_{\bar{\mu}^*}(mc^2\mathcal{I} - \beta E)\overline{\mathcal{V}}_{\bar{\mu}'}\overline{\Phi}^{(c)}_{\bar{\mu}'\kappa' m_j'}(E, \boldsymbol{r})$$
$$= -\mathrm{i}c\overline{h}\alpha\bar{\mu}^{-1}\,\mathrm{sign}(\zeta E \arg\bar{\mu})\delta(\arg\bar{\mu} - \arg\bar{\mu}')\delta_{\kappa\kappa'}\delta_{m_j m_j'} \tag{163}$$

$$\int_{\mathcal{R}^3} \mathrm{d}^3\boldsymbol{r}\, \overline{\Phi}^{(c)\dagger}_{\bar{\mu}^*\kappa m_j}(E, \boldsymbol{r})\overline{\mathcal{V}}^\dagger_{\bar{\mu}^*}(mc^2\mathcal{I} - \beta E)\overline{\mathcal{V}}_{\bar{\mu}'}\overline{\Phi}^{(r)}_{\bar{\mu}'\kappa' m_j'}(E, \boldsymbol{r}) = 0 \tag{164}$$

$$\int_{\mathcal{R}^3} \mathrm{d}^3\boldsymbol{r}\, \overline{\Phi}^{(r)\dagger}_{\bar{\mu}\kappa m_j}(E, \boldsymbol{r})\overline{\mathcal{V}}_{\bar{\mu}}(mc^2\mathcal{I} - \beta E)\overline{\mathcal{V}}_{\bar{\mu}'}\overline{\Phi}^{(c)}_{\bar{\mu}'\kappa' m_j'}(E, \boldsymbol{r}) = 0 \tag{165}$$

and

$$c^{-1}\overline{h}^{-1}\alpha^{-1}\sum_{\kappa m_j}\wp\int_{-\infty}^{\infty} \mathrm{d}\bar{\mu}\,\bar{\mu}^{-1}\,\mathrm{sign}[\zeta E(1 - \varepsilon^2\bar{\mu}^2)]\overline{\mathcal{V}}_{\bar{\mu}}\overline{\Phi}^{(r)}_{\bar{\mu}\kappa m_j}(E, \boldsymbol{r})$$

$$\times\overline{\Phi}^{(r)\dagger}_{\bar{\mu}\kappa m_j}(E,\boldsymbol{r}')\overline{\mathcal{V}}_{\bar{\mu}}(mc^2\mathcal{I}-\beta E)$$
$$+\mathrm{i}c^{-1}\overline{h}^{-1}\alpha^{-1}\sum_{\kappa m_j}\int_{-\pi}^{\pi}\mathrm{d}(\arg\bar{\mu})\,\bar{\mu}\,\mathrm{sign}(\zeta E\arg\bar{\mu})\overline{\mathcal{V}}_{\bar{\mu}}\overline{\Phi}^{(c)}_{\bar{\mu}\kappa m_j}(E,\boldsymbol{r})$$
$$\times\overline{\Phi}^{(c)\dagger}_{\bar{\mu}^*\kappa m_j}(E,\boldsymbol{r}')\overline{\mathcal{V}}^{\dagger}_{\bar{\mu}^*}(mc^2\mathcal{I}-\beta E)$$
$$=\delta(\boldsymbol{r}-\boldsymbol{r}')\mathcal{I} \tag{166}$$

where

$$\overline{\mathcal{V}}_{\bar{\mu}}=\begin{pmatrix} I & 0\\ 0 & \bar{\mu}^{-1}I\end{pmatrix}\equiv\mathcal{V}_{\mu}^{-1}. \tag{167}$$

From the results obtained thus far one may also deduce the second set of the orthogonality and closure relations for the three-dimensional Sturmians $\{\Phi_{\mu\kappa m_j}(E,\boldsymbol{r})\}$ and the radial Sturmians $\{S_{\mu\kappa}(x)\}$ and $\{T_{\mu\kappa}(x)\}$ which are *independent* from the relations found in section 4. On transforming equations (156), (160), (153) and (161) with the aid of the relations (138) one obtains, respectively,

$$\int_0^\infty \mathrm{d}x\,[S^{(r)}_{\mu\kappa}(x)S^{(r)}_{\mu'\kappa}(x)-\varepsilon^{-2}T^{(r)}_{\mu\kappa}(x)T^{(r)}_{\mu'\kappa}(x)]=-2\alpha\varepsilon^{-1}\mu\,\mathrm{sign}[\zeta(\mu^2-\varepsilon^2)]\,\delta(\mu-\mu') \tag{168}$$

$$\int_0^\infty \mathrm{d}x\,[S^{(c)}_{\mu\kappa}(x)S^{(c)}_{\mu'\kappa}(x)-\varepsilon^{-2}T^{(c)}_{\mu\kappa}(x)T^{(c)}_{\mu'\kappa}(x)]=-2\alpha\varepsilon^{-1}\mu\,\mathrm{sign}(\zeta\arg\mu)\,\delta(\arg\mu-\arg\mu') \tag{169}$$

$$\int_0^\infty \mathrm{d}x\,[S^{(r)}_{\mu\kappa}(x)S^{(c)}_{\mu'\kappa}(x)-\varepsilon^{-2}T^{(r)}_{\mu\kappa}(x)T^{(c)}_{\mu'\kappa}(x)]=0 \tag{170}$$

and

$$-\frac{\varepsilon}{2\alpha}\wp\int_{-\infty}^{\infty}\mathrm{d}\mu\,\mu^{-1}\,\mathrm{sign}[\zeta(\mu^2-\varepsilon^2)]\begin{pmatrix}S^{(r)}_{\mu\kappa}(x)\\ T^{(r)}_{\mu\kappa}(x)\end{pmatrix}\begin{pmatrix}S^{(r)}_{\mu\kappa}(x') & -\varepsilon^{-2}T^{(r)}_{\mu\kappa}(x')\end{pmatrix}$$
$$-\frac{\varepsilon}{2\alpha}\int_{-\pi}^{\pi}\mathrm{d}(\arg\mu)\,\mu^{-1}\,\mathrm{sign}(\zeta\arg\mu)\begin{pmatrix}S^{(c)}_{\mu\kappa}(x)\\ T^{(c)}_{\mu\kappa}(x)\end{pmatrix}\begin{pmatrix}S^{(c)}_{\mu\kappa}(x') & -\varepsilon^{-2}T^{(c)}_{\mu\kappa}(x')\end{pmatrix}$$
$$=\delta(x-x')I. \tag{171}$$

Similarly, on transforming equations (162)–(166) with the aid of relations (136), (139) and (140) one arrives at

$$\int_{\mathcal{R}^3}\mathrm{d}^3\boldsymbol{r}\,\Phi^{(r)\dagger}_{\mu\kappa m_j}(E,\boldsymbol{r})(mc^2\mathcal{I}-\beta E)\Phi^{(r)}_{\mu'\kappa' m_j'}(E,\boldsymbol{r})$$
$$=c\overline{h}\alpha\mu\,\mathrm{sign}[\zeta E(\mu^2-\varepsilon^2)]\,\delta(\mu-\mu')\delta_{\kappa\kappa'}\delta_{m_j m_j'} \tag{172}$$

$$\int_{\mathcal{R}^3}\mathrm{d}^3\boldsymbol{r}\,\Phi^{(c)\dagger}_{\mu^*\kappa m_j}(E,\boldsymbol{r})(mc^2\mathcal{I}-\beta E)\Phi^{(c)}_{\mu'\kappa' m_j'}(E,\boldsymbol{r})$$
$$=\mathrm{i}c\overline{h}\alpha\mu\,\mathrm{sign}(\zeta E\arg\mu)\delta(\arg\mu-\arg\mu')\delta_{\kappa\kappa'}\delta_{m_j m_j'} \tag{173}$$

$$\int_{\mathcal{R}^3}\mathrm{d}^3\boldsymbol{r}\,\Phi^{(c)\dagger}_{\mu^*\kappa m_j}(E,\boldsymbol{r})(mc^2\mathcal{I}-\beta E)\Phi^{(r)}_{\mu'\kappa' m_j'}(E,\boldsymbol{r})=0 \tag{174}$$

$$\int_{\mathcal{R}^3}\mathrm{d}^3\boldsymbol{r}\,\Phi^{(r)\dagger}_{\mu\kappa m_j}(E,\boldsymbol{r})(mc^2\mathcal{I}-\beta E)\Phi^{(c)}_{\mu'\kappa' m_j'}(E,\boldsymbol{r})=0 \tag{175}$$

and

$$c^{-1}\overline{h}^{-1}\alpha^{-1}\sum_{\kappa m_j}\wp\int_{-\infty}^{\infty}\mathrm{d}\mu\,\mu^{-1}\,\mathrm{sign}[\zeta E(\mu^2-\varepsilon^2)]\Phi^{(r)}_{\mu\kappa m_j}(E,\boldsymbol{r})\Phi^{(r)\dagger}_{\mu\kappa m_j}(E,\boldsymbol{r}')(mc^2\mathcal{I}-\beta E)$$

$$-\mathrm{i}c^{-1}\hbar^{-1}\alpha^{-1}\sum_{\kappa m_j}\int_{-\pi}^{\pi}\mathrm{d}(\arg\mu)\,\mu^{-1}\,\mathrm{sign}(\zeta E\arg\mu)\Phi^{(c)}_{\mu\kappa m_j}(E,\boldsymbol{r})$$
$$\times\Phi^{(c)\dagger}_{\mu^*\kappa m_j}(E,\boldsymbol{r}')(mc^2\mathcal{I}-\beta E)$$
$$=\delta(\boldsymbol{r}-\boldsymbol{r}')\,\mathcal{I}. \qquad (176)$$

6. Expansions in terms of the continuum Dirac–Coulomb Sturmian functions

Any sufficiently regular two-component spinor function $(F(x)\quad G(x))^{\top}$ (not to be confused with the function defined by equation (63)) defined in the interval $0 < x < \infty$ may be expanded in terms of either of the two radial Sturmian sets $\{(S_{\mu\kappa}(x)\quad T_{\mu\kappa}(x))^{\top}\}$ or $\{(\overline{S}_{\bar{\mu}\kappa}(x)\quad \overline{T}_{\bar{\mu}\kappa}(x))^{\top}\}$. The integral expansion in terms of the functions $\{(S_{\mu\kappa}(x)\quad T_{\mu\kappa}(x))^{\top}\}$ has the form

$$\begin{pmatrix}F(x)\\G(x)\end{pmatrix}=\wp\int_{-\infty}^{\infty}\mathrm{d}\mu\,\chi^{(r)}_{\mu\kappa}\begin{pmatrix}S^{(r)}_{\mu\kappa}(x)\\T^{(r)}_{\mu\kappa}(x)\end{pmatrix}+\int_{-\pi}^{\pi}\mathrm{d}(\arg\mu)\,\chi^{(c)}_{\mu\kappa}\begin{pmatrix}S^{(c)}_{\mu\kappa}(x)\\T^{(c)}_{\mu\kappa}(x)\end{pmatrix} \qquad (177)$$

where the expansion coefficients are given by (cf equations (168)–(170))

$$\chi^{(r)}_{\mu\kappa}=-\frac{\varepsilon}{2\alpha}\mu^{-1}\,\mathrm{sign}[\zeta(\mu^2-\varepsilon^2)]\int_0^{\infty}\mathrm{d}x\,[S^{(r)}_{\mu\kappa}(x)F(x)-\varepsilon^{-2}T^{(r)}_{\mu\kappa}(x)G(x)] \qquad (178)$$

$$\chi^{(c)}_{\mu\kappa}=-\frac{\varepsilon}{2\alpha}\mu^{-1}\,\mathrm{sign}(\zeta\arg\mu)\int_0^{\infty}\mathrm{d}x\,[S^{(c)}_{\mu\kappa}(x)F(x)-\varepsilon^{-2}T^{(c)}_{\mu\kappa}(x)G(x)]. \qquad (179)$$

The expansion of $(F(x)\quad G(x))^{\top}$ in terms of the Sturmians $\{(\overline{S}_{\bar{\mu}\kappa}(x)\quad \overline{T}_{\bar{\mu}\kappa}(x))^{\top}\}$ is

$$\begin{pmatrix}F(x)\\G(x)\end{pmatrix}=\wp\int_{-\infty}^{\infty}\mathrm{d}\bar{\mu}\,\bar{\chi}^{(r)}_{\bar{\mu}\kappa}\begin{pmatrix}\overline{S}^{(r)}_{\bar{\mu}\kappa}(x)\\\overline{T}^{(r)}_{\bar{\mu}\kappa}(x)\end{pmatrix}+\int_{-\pi}^{\pi}\mathrm{d}(\arg\bar{\mu})\,\bar{\chi}^{(c)}_{\bar{\mu}\kappa}\begin{pmatrix}\overline{S}^{(c)}_{\bar{\mu}\kappa}(x)\\\overline{T}^{(c)}_{\bar{\mu}\kappa}(x)\end{pmatrix} \qquad (180)$$

and it follows from equations (141)–(143) that the coefficients $\bar{\chi}^{(r)}_{\bar{\mu}\kappa}$ and $\bar{\chi}^{(c)}_{\bar{\mu}\kappa}$ are

$$\bar{\chi}^{(r)}_{\bar{\mu}\kappa}=\bar{\mu}^{-2}\,\mathrm{sign}(1-\varepsilon^2\bar{\mu}^2)\int_0^{\infty}\mathrm{d}x\,\frac{|Z|}{x}[\overline{S}^{(r)}_{\bar{\mu}\kappa}(x)F(x)-\overline{T}^{(r)}_{\bar{\mu}\kappa}(x)G(x)] \qquad (181)$$

$$\bar{\chi}^{(c)}_{\bar{\mu}\kappa}=-\,\mathrm{sign}(\arg\bar{\mu})\int_0^{\infty}\mathrm{d}x\,\frac{|Z|}{x}[\overline{S}^{(c)}_{\bar{\mu}\kappa}(x)F(x)-\overline{T}^{(c)}_{\bar{\mu}\kappa}(x)G(x)]. \qquad (182)$$

Similarly, any sufficiently regular four-component spinor function $\Psi(\boldsymbol{r})$ defined in $\mathcal{R}^3$ may be expanded in either of the sets $\{\Phi_{\mu\kappa m_j}(E,\boldsymbol{r})\}$ or $\{\overline{\Phi}_{\bar{\mu}\kappa m_j}(E,\boldsymbol{r})\}$. One has

$$\Psi(\boldsymbol{r})=\sum_{\kappa m_j}\wp\int_{-\infty}^{\infty}\mathrm{d}\mu\,\chi^{(r)}_{\mu\kappa m_j}\Phi^{(r)}_{\mu\kappa m_j}(E,\boldsymbol{r})+\sum_{\kappa m_j}\int_{-\pi}^{\pi}\mathrm{d}(\arg\mu)\,\chi^{(c)}_{\mu\kappa m_j}\Phi^{(c)}_{\mu\kappa m_j}(E,\boldsymbol{r}) \qquad (183)$$

where the coefficients $\chi^{(r)}_{\mu\kappa m_j}$ and $\chi^{(c)}_{\mu\kappa m_j}$ are found from equations (172)–(175) to be

$$\chi^{(r)}_{\mu\kappa m_j}=c^{-1}\hbar^{-1}\alpha^{-1}\mu^{-1}\,\mathrm{sign}[\zeta E(\mu^2-\varepsilon^2)]\int_{\mathcal{R}^3}\mathrm{d}^3\boldsymbol{r}\,\Phi^{(r)\dagger}_{\mu\kappa m_j}(E,\boldsymbol{r})(mc^2\mathcal{I}-\beta E)\Psi(\boldsymbol{r}) \qquad (184)$$

$$\chi^{(c)}_{\mu\kappa m_j}=-\mathrm{i}c^{-1}\hbar^{-1}\alpha^{-1}\mu^{-1}\,\mathrm{sign}(\zeta E\arg\mu)\int_{\mathcal{R}^3}\mathrm{d}^3\boldsymbol{r}\,\Phi^{(c)\dagger}_{\mu^*\kappa m_j}(E,\boldsymbol{r})(mc^2\mathcal{I}-\beta E)\Psi(\boldsymbol{r}) \qquad (185)$$

and

$$\Psi(\boldsymbol{r})=\sum_{\kappa m_j}\wp\int_{-\infty}^{\infty}\mathrm{d}\bar{\mu}\,\bar{\chi}^{(r)}_{\bar{\mu}\kappa m_j}\overline{\Phi}^{(r)}_{\bar{\mu}\kappa m_j}(E,\boldsymbol{r})+\sum_{\kappa m_j}\int_{-\pi}^{\pi}\mathrm{d}(\arg\bar{\mu})\,\bar{\chi}^{(c)}_{\bar{\mu}\kappa m_j}\overline{\Phi}^{(c)}_{\bar{\mu}\kappa m_j}(E,\boldsymbol{r}) \qquad (186)$$

where the coefficients $\bar{\chi}^{(r)}_{\bar{\mu}\kappa m_j}$ and $\bar{\chi}^{(c)}_{\bar{\mu}\kappa m_j}$ are found from equations (145)–(148) to be

$$\bar{\chi}^{(r)}_{\bar{\mu}\kappa m_j} = \bar{\mu}^{-2}\,\mathrm{sign}(1-\varepsilon^2\bar{\mu}^2)\int_{\mathcal{R}^3} \mathrm{d}^3\boldsymbol{r}\,\frac{|Z|}{r}\,\overline{\Phi}^{(r)\dagger}_{\bar{\mu}\kappa m_j}(E,\boldsymbol{r})\beta\Psi(\boldsymbol{r}) \tag{187}$$

$$\bar{\chi}^{(c)}_{\bar{\mu}\kappa m_j} = \mathrm{i}\,\mathrm{sign}(\arg\bar{\mu})\int_{\mathcal{R}^3} \mathrm{d}^3\boldsymbol{r}\,\frac{|Z|}{r}\,\overline{\Phi}^{(c)\dagger}_{\bar{\mu}^*\kappa m_j}(E,\boldsymbol{r})\beta\Psi(\boldsymbol{r}). \tag{188}$$

7. Conclusions

Two aims have been achieved in this work. First, we have investigated properties of the continuum Schrödinger–Coulomb Sturmian functions. The functions have been constructed by solving an appropriate eigenvalue problem, properly normalized and shown to form a non-enumerable set with elements labelled by real eigenvalues μ covering the whole real axis, $-\infty < \mu < \infty$. The latter result resolves a disagreement between Khristenko [3], who asserted that eigenvalues μ ranged from $-\infty$ to $+\infty$ (which agrees with our result), and Blinder [5, 6], who claimed that eigenvalues μ were restricted to the real positive half-axis.

The second aim achieved in this paper was the construction of two types of continuum Dirac–Coulomb Sturmians. It has been shown that both types of the Dirac–Coulomb Sturmians are closely related and may be found as solutions of generalized Sturm–Liouville problems for two coupled first-order differential equations, augmented by appropriate boundary conditions, with eigenvalues chosen in rather unusual ways. It was shown that eigenvalue spectra for both problems consist of the real axis with zero excluded plus relevant circumferences in the complex plane centred at zero. Occurrence of the complex eigenvalues is the consequence of the way in which the eigenvalues in the defining Sturm–Liouville problems are chosen. Another peculiarity encountered in the course of investigation of properties of both types of the continuum Dirac–Coulomb Sturmian functions is the existence of two different kinds of the orthogonality and closure relations obeyed by these functions. This feature is due to the relationship found between the two types of the Dirac–Coulomb Sturmians.

The continuum non-relativistic and relativistic Coulomb Sturmian functions may find applications in analysing those atomic phenomena in which free electrons interact with charged atomic targets, for example, in electron–ion collisions or in atomic photoionization. In some theoretical methods used to describe such processes one employs the Coulomb Green function for continuum eigenenergies [17–20]. Use of the continuum Coulomb Sturmian functions described in this work offers a possibility to construct an integral representation of the Coulomb Green function. It seems that by employing the powerful method of contour integration one may transform that representation to a form which will be equally useful in applications as forms known before [17–20]. We shall consider this problem in a later publication.

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Appendix A. The Whittaker function $M_{\eta\gamma}(z)$

In this appendix we summarize those properties of the Whittaker function of the first kind, $M_{\eta\gamma}(z)$, which have been useful in studying properties of the continuum Coulomb Sturmian functions. A more comprehensive treatment of the Whittaker function may be found in [10, 11].

The function $M_{\eta\gamma}(z)$ is defined in terms of the confluent hypergeometric function

$$ {}_1F_1(a;b;z) = 1 + \frac{a}{b}\frac{z}{1!} + \frac{a(a+1)}{b(b+1)}\frac{z^2}{2!} + \frac{a(a+1)(a+2)}{b(b+1)(b+2)}\frac{z^3}{3!} + \cdots \tag{189}$$

in the following way

$$M_{\eta\gamma}(z) = z^{\gamma+1/2}\mathrm{e}^{-z/2}\,{}_1F_1(\gamma + \tfrac{-}{\eta}; 2\gamma+1; z). \tag{190}$$

It is a solution of the Whittaker differential equation

$$\left[\frac{\mathrm{d}^2}{\mathrm{d}z^2} - \frac{\gamma^2 - \frac{1}{4}}{z^2} + \frac{\eta}{z} - \frac{1}{4}\right] M_{\eta\gamma}(z) = 0. \tag{191}$$

In the vicinity of the regular singular point $z = 0$ the function $M_{\eta\gamma}(z)$ behaves as

$$M_{\eta\gamma}(z) \xrightarrow{z\to 0} z^{\gamma+1/2}\left(1 - \frac{\eta}{2\gamma+1}z\right). \tag{192}$$

For large values of the argument the function $M_{\eta\gamma}(z)$ has the asymptotic expansion

$$M_{\eta\gamma}(z) \xrightarrow{|z|\to\infty} z^{\gamma+1/2}\mathrm{e}^{-z/2}\left[\frac{\Gamma(2\gamma+1)}{\Gamma(\gamma+\frac{1}{2}+\eta)}(-z)^{-\gamma-1/2+\eta} + \frac{\Gamma(2\gamma+1)}{\Gamma(\gamma+\frac{1}{2}-\eta)}z^{-\gamma-1/2-\eta}\mathrm{e}^{z}\right] \tag{193}$$

valid provided

$$|\arg(-z)| < \pi \qquad \text{and} \qquad |\arg z| < \pi. \tag{194}$$

The restriction (194) is satisfied if we define

$$-z = \mathrm{e}^{\mathrm{i}\pi\Delta(z)}z \qquad \Delta(z) = \begin{cases} -1 & \text{for } 0 < \arg z < \pi \\ +1 & \text{for } -\pi < \arg z < 0. \end{cases} \tag{195}$$

It follows from the relation (190), the definition (189) and the Kummer identity

$${}_1F_1(a;b;z) = \mathrm{e}^{z}\,{}_1F_1(b-a;b;-z) \tag{196}$$

that

$$M_{\eta\gamma}(z) = \mathrm{e}^{-\mathrm{i}\pi(\gamma+1/2)\Delta(z)}M_{-\eta\gamma}(-z). \tag{197}$$

The following complex conjugation formula stems from the relation (190), the definition (189) and the Kummer identity (196)

$$[M_{\alpha+\mathrm{i}\beta,\gamma}(\pm\mathrm{i}x)]^* = \mathrm{e}^{\mp\mathrm{i}\pi(\gamma+1/2)}M_{-\alpha+\mathrm{i}\beta,\gamma}(\pm\mathrm{i}x) \qquad (x > 0) \tag{198}$$

where x is real and positive while α, β and γ are real.

The recurrence relations

$$M_{\eta,\gamma+1/2}(z) = (2\gamma+1)z^{-1/2}M_{\eta-1/2,\gamma}(z) - (2\gamma+1)z^{-1/2}M_{\eta+1/2,\gamma}(z) \tag{199}$$

$$M_{\eta,\gamma-1/2}(z) = \frac{\gamma-\eta}{2\gamma}z^{-1/2}M_{\eta-1/2,\gamma}(z) + \frac{\gamma+\eta}{2\gamma}z^{-1/2}M_{\eta+1/2,\gamma}(z) \tag{200}$$

have been useful in obtaining the representations (78) and (79) of the radial Sturmians from those given by equations (76) and (77).

Appendix B. Coulomb versus non-Coulomb Sturmians

Let us consider a class of spherically symmetric real potentials $V(r)$ such that

$$\lim_{r\to 0} rV(r) = \text{constant} \qquad \lim_{r\to\infty} r^2 V(r) = \text{constant}' \tag{201}$$

(note that potentials vanishing asymptotically as the Coulomb potential do not fall into this class). For a given potential $V(r)$ from the class considered we define the non-relativistic positive-energy radial Sturmians $\{P_{\mu_l l}(r)\}$ as those solutions of the differential equation

$$\left[\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} - \mu_l U(r) + \lambda^2\right] P_{\mu_l l}(r) = 0 \qquad (0 \leqslant r < \infty) \tag{202}$$

which obey the boundary conditions

$$P_{\mu_l l}(r) \overset{l}{\sim} r \to 0 r^{l+1} \qquad P_{\mu_l l}(r) \text{ bounded for } r \to \infty. \tag{203}$$

In equation (202) $U(r) = 2mV(r)/\hbar^2$, $\lambda^2 = 2mE/\hbar^2 > 0$ is a parameter and μ_l is an eigenvalue. It is known [21] that problem (202) and (203) has a continuous spectrum of non-degenerate real eigenvalues $-\infty < \mu_l < \infty$ and that the eigenfunctions behave asymptotically as

$$P_{\mu_l l}(r) \overset{r\to\infty}{\longrightarrow} B_{\mu_l l} \sin(\lambda r - \frac{1}{2}\pi l + \delta_l(\mu_l)) \tag{204}$$

where $B_{\mu_l l}$ is a normalization factor and $\delta_l(\mu_l)$ (not to be confused with the Kronecker delta symbol or the Dirac delta function) is a phase shift. The question of orthogonality of the Sturmians $\{P_{\mu_l l}(r)\}$ may be investigated in a manner analogous to that we have adopted in section 2. We change the independent variable from r to r' and consider two differential equations of the form (202) obeyed by the functions $P_{\mu_l l}(r')$ and $P_{\mu_l' l}(r')$ corresponding to the eigenvalues μ_l and μ_l', respectively. On premultiplying the first equation by $P_{\mu_l' l}(r')$, the second by $P_{\mu_l l}(r')$, subtracting, integrating from $r' = 0$ to $r' = r$ and utilizing the boundary condition satisfied by the Sturmians at $r' = 0$ we obtain

$$(\mu_l - \mu_l') \int_0^r dr'\, U(r') P_{\mu_l l}(r') P_{\mu_l' l}(r') = P_{\mu_l' l}(r) \frac{dP_{\mu_l l}(r)}{dr} - P_{\mu_l l}(r) \frac{dP_{\mu_l' l}(r)}{dr}. \tag{205}$$

For large values of r the Sturmians on the right-hand side of equation (205) may be replaced by their asymptotic forms (204). Passing to the limit $r \to \infty$ we find

$$\int_0^\infty dr\, U(r) P_{\mu_l l}(r) P_{\mu_l' l}(r) = -\lambda B_{\mu_l l} B_{\mu_l' l} \frac{\sin[\delta_l(\mu_l) - \delta_l(\mu_l')]}{\mu_l - \mu_l'}. \tag{206}$$

From this result one infers that for potentials which vanish asymptotically faster than the Coulomb potential positive-energy Sturmians are *not* orthogonal in the sense in which the Coulomb Sturmians $\{S_{\mu_l l}(2\lambda r)\}$ are. For, if the functions $\{P_{\mu_l l}(r)\}$ could be orthogonalized to the delta function $\delta(\mu_l - \mu_l')$, the right-hand side of equation (206) would be singular for $\mu_l = \mu_l'$. However, considering the fraction appearing on the right-hand side of equation (206) which is the only term which could possibly give rise to the singularity, one finds

$$\frac{\sin[\delta_l(\mu_l) - \delta_l(\mu_l')]}{\mu_l - \mu_l'} \overset{\mu_l' \to \mu_l}{\longrightarrow} \frac{\partial \delta_l(\mu_l)}{\partial \mu_l}. \tag{207}$$

In general, the derivative on the right-hand side of equation (207) is finite and this implies that the positive-energy non-Coulomb Sturmians are not orthogonal in the sense of the Dirac delta function. This fact diminishes the value of such functions for potential applications in quantum mechanical problems.

Comparing the right-hand sides of equations (23) and (207) one notes that the exceptional position which the Coulomb Sturmians occupy among other functions of that sort is due to the long-range nature of the Coulomb potential resulting in the logarithmic phase $\eta \ln 2\lambda r$ appearing in the asymptotic form of the eigenfunctions. It is just this factor which causes orthogonality of the Coulomb Sturmians in the sense of equation (25).

Analogous considerations may be carried out in the relativistic case.

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