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# Two-body Coulomb wavefunctions as kernel for alternative integral transformations

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## Abstract

In this paper we investigate different representations of an arbitrary function in terms of two-body Coulomb eigenfunctions. We discuss the standard energy basis in spherical and parabolic coordinates with the purpose of remarking explicitly that two additional parameters appear both in the Schrödinger equation and in the wavefunctions: the charge and the angular momentum. We introduce the charge and generalized angular momentum Sturmian function representations, which result when the charge or the angular momentum is used as the eigenvalue in the Coulomb Schrödinger equation, respectively. We present the connection between the generalized angular momentum representation and the Kontorovich–Lebedev transform. Finally, we extend the angular momentum representation to six dimensions, which is suitable for further applications in the three-body Coulomb problem.

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## 1. Introduction

The standard way of theoretically studying the properties of a wide variety of atomic and molecular systems is by using functional basis set for representing the physical magnitudes involved in the phenomena under analysis. According to the mathematical structure of quantum mechanics, each physical magnitude has a Hermitian operator associated and then its eigenfunctions become the natural basis set to be used. The most common basis set uses the *energy eigenfunctions*, i.e., the eigenfunctions of the Hamiltonian. However, in some cases the energy eigenfunctions are not the most convenient ones and alternative basis sets are necessary.

For years an energy eigenfunction representation has been known for the two-body Coulomb Green function, however it has not been used because of the inconvenience in dealing with it [1]. The so-called Sturmian functions have been developed as alternative basis set functions. The underlying idea is that the energy is considered in the Sturmian functions as a fixed parameter and that the energy wave equation is solved considering some other parameter as the eigenvalue [2, 3].

The energy eigenfunctions result by solving the Schrödinger equation considering the energy  $E$  as the eigenvalue of the problem. However, the charge of the particles or, after variable separation, the angular momentum, can also be considered as the eigenvalue in the wave equation. In connection with the two-body Coulomb problem, the charge Sturmian functions have been introduced as the solution of the 'radial' Schrödinger equation with particular boundary conditions using the charge as the eigenvalue of the problem [2, 3]. In that case, the energy and other parameters appearing in the differential equation are considered constants. This property is useful in many calculations where the two-body Coulomb Green functions are needed (see [1] and references therein). Other Sturmian functions have also been defined when dealing with three-body Coulomb problems [4–9] and also when short-range interactions are considered [10].

In the two-body Coulomb problem case, charge Sturmians in spherical coordinates are properly defined when the energy  $E$  is less than zero. However a discrepancy can be found in the literature when defining these functions for  $E > 0$ . The main problem seems to be connected with the nature of the spectra of charge eigenvalues: Ovchinnikov and Macek [6] and Shakeshaft [11] found discrete spectra while Blinder [12] and Szmytkowski [13] obtained continuous ones. When solving the radial Sturmian eigenvalue equation, Ovchinnikov and Szmytkowski used the same boundary condition at the origin, but different boundary conditions at infinity. This led to Sturmian functions with different asymptotic behaviour. Ovchinnikov's Sturmians satisfy a mixed boundary condition where a linear combination of the Sturmian function and its derivative are restricted to be zero. Therefore, the function itself is not bounded at infinity but the eigenvalue spectra are discrete. On the other hand, Szmytkowski solved the Sturmian eigenequation with the condition of having a bounded function at infinity, giving rise to a continuous eigenvalue spectrum. Shakeshaft's results are in agreement with those of Ovchinnikov. Szmytkowski's results partially agree with those of Blinder, but Blinder's definition leads to half of the spectrum found by Szmytkowski. One of the aims of this paper is to show that a set of charge Sturmians can be defined as having continuous spectra in agreement with Szmytkowski. An inverse transformation considering Laguerre functions as the kernel will be used for that purpose. The method gives us also the possibility of defining a set of charge Sturmians in parabolic coordinates.

The second purpose of this paper is to introduce a new two-body Coulomb Sturmian. To this end we use an inverse transformation with a kernel represented in terms of Meijer's functions. In these functions, the energy and charge are considered constants, but a generalized angular momentum is considered the eigenvalue.

In section 2 we give the main equations related to the energy eigenfunctions. We review the eigenequation in spherical and parabolic coordinates and show how to get a representation for an arbitrary function based on the theory of generating functions. In section 3 we derive a set of charge Sturmian functions in spherical and parabolic coordinates. We start from an inverse transformation derived from the theory of generating functions. We show that there is only one set of functions for both the discrete and continuous energy spectra, and the eigenvalues of these functions belong to a continuum spectrum. The energy (or alternatively the momentum) is a parameter in these functions, and can be analytically extended from the positive to the negative axis. This will be used to establish the connection with the discrete

spectrum functions. In section 4 we present the *angular momentum Sturmian* functions. Two alternative basis functions are derived, based on the irregular and the regular solutions of the two-body Coulomb problem. The eigenvalues associated with these basis functions belong to continuum spectra. In the representation to be discussed, the energy (or momentum) also enters as a parameter, and can also be extended to the complex plane to deal with both positive and negative energies. We discuss the connection of this basis with the well-known Kontorovich–Lebedev transformation. In section 5 the angular momentum Sturmian basis is applied to write the approximate solutions of the three-body Coulomb problem [14–17]. We analyse the asymptotic limits in Redmond’s region (when the three particles are far apart) and remark the equivalence to a Mellin–Barnes integral representation in the condensation region. We summarize the results, and discuss further work in the last section. Atomic units are used unless otherwise stated.

## 2. General considerations

The two-body Schrödinger equation for the Coulomb potential is

$$\left[ -\frac{1}{2\mu}\nabla^2 - \frac{Z}{r} - E \right] \Phi(\mathbf{r}) = 0 \quad (1)$$

where  $E = k^2/2\mu$  is the energy,  $k$  is the relative momentum between the particles,  $Z$  represents the product of the charges and  $\mu$  is the reduced mass of the particles. This equation can be solved by variable separation in three different sets of coordinates: spherical, parabolic and prolate spheroidal [18]. In this paper we consider the first two.

Equation (1) is usually defined as an eigenvalue problem where  $\Phi(\mathbf{r})$  and  $E$ , or the momentum  $k$ , are defined as the eigenfunction and eigenvalue, respectively. This problem is thoroughly studied in different textbooks [18, 19, 23], so we summarize the main results in spherical and parabolic coordinates only.

### 2.1. Spherical coordinates

Once equation (1) is written in spherical coordinates and the separation of variables is performed by writing the wavefunction as the product of an angular and a radial part

$$\Phi(r, \theta, \phi) = R_{k,l}(r)Y_l^m(\theta, \phi) \quad (2)$$

the following equation results for the radial part  $R_{k,l}(r)$ :

$$\left[ \frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} - \frac{l(l+1)}{r^2} + \frac{2\mu Z}{r} + k^2 \right] R_{k,l}(r) = 0. \quad (3)$$

In equation (2),  $l(l+1)$  and  $Y_l^m(\theta, \phi)$  represent the eigenvalue and eigenfunction of the angular momentum  $\mathbf{L}^2$ , respectively [19].

From equation (3), we see that, besides the reduced mass  $\mu$ , there are three other parameters: the momentum  $k$ , the charge  $Z$  and the angular momentum  $l$ . If the momentum  $k$  is considered the eigenvalue of the problem, the other two parameters remain constants when solving the equation. The eigensolutions  $R_{k,l}(r)$  corresponding to the continuous spectrum of

$E$  (or  $k$ ) are

$$\begin{aligned} R_{k,l}(r) &= \frac{2k|\Gamma(l+1-i\beta)|}{\Gamma(2l+2)} e^{\frac{\pi}{2}\beta} (2ikr)^l e^{-ikr} F[l+1+i\beta, 2l+2, 2ikr] \\ &= \frac{2k|\Gamma(l+1-i\beta)|}{\Gamma(2l+2)} e^{\frac{\pi}{2}\beta} \frac{1}{r} M_{-i\beta, l+1/2}(2ikr) \end{aligned} \quad (4)$$

where  $\beta = \frac{Z\mu}{k}$  is the Sommerfeld parameter.  $F[b, c, z]$  represents the Kummer function [21] and  $M_{a,c}(z)$  the regular Whittaker function [22]. In  $R_{k,l}(r)$ , the eigenvalue  $k$  appears not only in the argument of the Whittaker function, but also in the first parameter.

The eigensolutions of equation (3) corresponding to the discrete spectrum associated with  $E \leq 0$  are

$$\begin{aligned} R_{n,l}(r) &= \frac{2}{n^2\Gamma(2l+2)} \sqrt{\frac{\Gamma(n+l+1)}{\Gamma(n-l)}} \left(\frac{2Z\mu}{n}r\right)^l e^{-\frac{Z\mu}{n}r} F\left[l+1-n, 2l+2, \frac{2Z\mu}{n}r\right] \\ &= \frac{2}{n^2\Gamma(2l+2)} \sqrt{\frac{\Gamma(n+l+1)}{\Gamma(n-l)}} \frac{1}{r} M_{n, l+1/2}\left(\frac{2Z\mu}{n}r\right). \end{aligned} \quad (5)$$

The set of functions  $\{R_{n,l}(r), R_{k,l}(r)\}$  constitutes a set of doubly orthogonal functions, with orthogonality and closure relations given by

$$\int_0^\infty R_{k',l}(r) R_{k,l}(r) r^2 dr = 2\pi \delta(k-k') \quad (6)$$

$$\int_0^\infty R_{n',l}(r) R_{n,l}(r) r^2 dr = \delta_{n,n'} \quad (7)$$

and

$$\sum_{n=1}^\infty R_{n,l}(r') R_{n,l}(r) + \int_0^\infty R_{k,l}(r') R_{k,l}(r) k^2 dk = 2\pi \delta(r-r'). \quad (8)$$

The functions (4) and (5) can be used to write any arbitrary function  $\Psi(r)$ , belonging in general to an  $\mathbf{L}^2$  space of functions. In terms of these energy eigenfunctions, we have the expansion

$$\Psi(r) = \sum_{n=0}^\infty a_n R_{n,l}(r) + \int_0^\infty A(k) R_{k,l}(r) k^2 dk \quad (9)$$

where the coefficients  $a_n$  and  $A(k)$  are defined in terms of the basis functions  $\{R_{n,l}(r), R_{k,l}(r)\}$  by

$$a_n = \int_0^\infty \Psi(r) R_{n,l}(r) r^2 dr \quad (10)$$

and

$$A(k) = \int_0^\infty \Psi(r) R_{k,l}(r) r^2 dr. \quad (11)$$

## 2.2. Parabolic coordinates

A set of energy basis functions can be obtained when equation (1) is separated into parabolic coordinates  $\{\xi, \eta, \phi\}$  [18, 19]:

$$\left\{ \frac{4}{\xi + \eta} \left( \frac{\partial}{\partial \xi} \left( \xi \frac{\partial}{\partial \xi} \right) + \frac{\partial}{\partial \eta} \left( \eta \frac{\partial}{\partial \eta} \right) \right) + \frac{1}{\xi \eta} \frac{\partial^2}{\partial \phi^2} + \frac{4Z\mu}{\xi + \eta} + k^2 \right\} \Phi(\xi, \eta, \phi) = 0. \quad (12)$$

If the wavefunction  $\Phi(\xi, \eta, \phi)$  is written as the product of the eigenfunction  $e^{im\phi}$  of the angular momentum projection  $L_z^2$  and a product of functions in  $\xi$  and  $\eta$

$$\Phi(\xi, \eta, \phi) = e^{im\phi} \frac{1}{\sqrt{\xi\eta}} \varphi_{1,k,m}(\xi) \varphi_{2,k,m}(\eta) \quad (13)$$

equation (12) separates as

$$\begin{aligned} \left[ \frac{d^2}{d\xi^2} + \left( \frac{k^2}{4} + \frac{\lambda_1\mu}{\xi} + \frac{1-m^2}{4\xi} \right) \right] \varphi_{1,k,m}(\xi) &= 0 \\ \left[ \frac{d^2}{d\eta^2} + \left( \frac{k^2}{4} + \frac{\lambda_2\mu}{\eta} + \frac{1-m^2}{4\eta^2} \right) \right] \varphi_{2,k,m}(\eta) &= 0. \end{aligned} \quad (14)$$

The angular momentum projection eigenvalue is represented by  $m$ , while  $\lambda_1$  and  $\lambda_2$  are the separation constants that satisfy the relation  $\lambda_1 + \lambda_2 = Z$ .

As in the case of radial equation (3), there are three parameters in (14): the momentum  $k$ , the angular momentum  $m$  and a charge represented by  $\lambda_i$ . When the energy  $E$  (or the momentum  $k$ ) is considered as the eigenvalue of the problem, equations (14) can be solved in terms of the regular Whittaker functions  $M_{a,c}(z)$  as follows:

$$\varphi_{1,k,m}(\xi) = N_{\beta_1,m} M_{-i\beta_1, \frac{m}{2}}(ik\xi) \quad \varphi_{2,k,m}(\eta) = N_{\beta_2,m} M_{-i\beta_2, \frac{m}{2}}(ik\eta) \quad (15)$$

where the normalization factor is ( $j = 1, 2$ )

$$N_{\beta_j,m} = \frac{\Gamma\left(\frac{1}{2} + i\beta_j + \frac{m}{2}\right)}{\Gamma(m+1)} \quad (16)$$

and depends on the momentum through the Sommerfeld parameter  $\beta_i = \frac{\lambda_i\mu}{k}$ .

In terms of the irregular Whittaker functions the solutions read

$$\overline{\varphi}_{k,m}^{(1)}(\xi) = W_{-i\beta_1, \frac{m}{2}}(ik\xi) \quad \overline{\varphi}_{k,m}^{(2)}(\eta) = W_{-i\beta_2, \frac{m}{2}}(ik\eta). \quad (17)$$

The eigenfunctions corresponding to the discrete energy spectrum in each of the parabolic coordinates  $\xi$  and  $\eta$  are

$$\begin{aligned} \varphi_{1,n_1,m}(\xi) &= \frac{1}{\Gamma(m+1)} \sqrt{\frac{\Gamma(n_1+m+1)}{\Gamma(n_1+1)}} M_{n_1+\frac{m+1}{2}, \frac{m}{2}}\left(\frac{Z\mu}{n_1}\xi\right) \\ \varphi_{2,n_2,m}(\eta) &= \frac{1}{\Gamma(m+1)} \sqrt{\frac{\Gamma(n_2+m+1)}{\Gamma(n_2+1)}} M_{n_2+\frac{m+1}{2}, \frac{m}{2}}\left(\frac{Z\mu}{n_2}\eta\right). \end{aligned} \quad (18)$$

The eigenfunctions  $\{\varphi_{1,n_1,m}(\xi), \varphi_{2,n_2,m}(\eta)\}$  constitute a complete set of orthogonal functions. Then, any arbitrary function  $\Psi(\eta)$  can be written as

$$\Psi(\eta) = \sum_{n=0}^{\infty} b_n \varphi_{2,n,m}(\eta) + \int_0^{\infty} B(k) \varphi_{2,k,m}(\eta) dk \quad (19)$$

where the coefficients  $b_n$  and  $B(k)$  are obtained by using the orthogonality properties of  $\varphi_{2,n,m}(\eta)$  and  $\varphi_{2,k,m}(\eta)$ ,

$$b_n = \int_0^{\infty} \varphi_{2,n,m}(\eta) \Psi(\eta) \frac{1}{\eta} d\eta \quad (20)$$

$$B(k) = \int_0^\infty \varphi_{2,k,m}(\eta) \Psi(\eta) \frac{1}{\eta} d\eta. \quad (21)$$

A similar analysis can be performed for functions depending on  $\xi$ . The set of functions in  $\xi$  and  $\eta$  is a complete basis and then these results can be applied to any function  $\Psi(\xi, \eta)$ .

This review shows explicitly that three parameters are involved in each of the equations, both in spherical and in parabolic coordinates. Then, it is possible to solve the same set of equations in two alternative ways. We can choose the charge  $Z$  (or the  $\lambda$  in parabolic coordinates) or the angular momentum  $l$  (or  $m$  in parabolic coordinates) as eigenvalues.

### 2.3. Generating functions

The method discussed before is based on the theory of differential equations. Another way to obtain the set of functions is to use the theory of generating functions. The most frequent way of introducing the generating function is by means of the relation

$$\Delta(z, t) = \sum_{s=0}^{\infty} \Lambda_s(z) t^s. \quad (22)$$

$\Delta(z, t)$  is called the generating function for the set of functions  $\Lambda_s(z)$ . The name generating function was introduced by Laplace in 1812 [20]. The definition is not restricted to the case of series; also the concept of ‘generating function’ was introduced for integrals. The generalization of equation (22) is

$$\Delta(z, t) = \int_0^\infty t^s \Lambda(s, z) ds. \quad (23)$$

One of the most important examples of these integrals is the Laplace transformation [21].

The whole theory of orthogonal polynomials can be derived from the theory of generating functions. All the orthogonal polynomials (Laguerre, Hermite, Legendre, etc), as well as their properties can be obtained from their generating functions. Two important examples of generating functions connected with what we are going to discuss in the following sections are

- The Laguerre polynomials  $L_n^\alpha(x)$

$$\frac{1}{(1-t)^{\alpha+1}} e^{-\frac{xt}{1-t}} = \sum_{n=0}^{\infty} t^n \frac{L_n^\alpha(x)}{\Gamma(\alpha+1+n)}. \quad (24)$$

- Generalized Neumann polynomials  $A_{\beta, \mu/2+s, s}$  [22]

$$\frac{z^{\frac{\mu+1}{2}}}{t-z} = \sum_{s=0}^{\infty} A_{\beta, \mu/2+s, s}(t) M_{\beta, \mu/2+s}(z) \quad |t| > |z|. \quad (25)$$

The theory of generating functions allows us to obtain a representation of an arbitrary function  $\Psi(z)$  in terms of the basis functions  $\Lambda_s(z)$  and/or  $\Lambda(s, z)$  [24].

Let us assume that the function  $\Psi(z)$  is single valued and regular within and on the boundary of a circle  $K$  around the origin. Then, for every point  $z$  within the circle, Cauchy’s theorem gives

$$z^{\frac{\mu+1}{2}} \Psi(z) = \frac{1}{2\pi i} \int_K \frac{\Psi(t) z^{\frac{\mu+1}{2}}}{t-z} dt. \quad (26)$$

Using relation (25) and interchanging the order of integration and summation (which is allowed because of its uniform convergence), we obtain

$$z^{\frac{\mu+1}{2}} \Psi(z) = \sum_{s=0}^{\infty} a_s M_{\beta, \mu/2+s}(z) \quad (27)$$

where the coefficients  $a_s$  are

$$a_s = \frac{1}{2\pi i} \int_K A_{\beta, \mu/2+s, s}(t) \Psi(t) dt. \quad (28)$$

A similar procedure can be followed to get an integral representation of a general function  $\Psi(z)$  based on any of the integral generating functions.

### 3. Charge Sturmians

The two-body charge Coulomb Sturmians with energies less than zero or with discrete charge spectrum were all given in terms of Laguerre polynomials, both in spherical [1, 3, 6, 11] and parabolic coordinates [25]. The properties of these Sturmian functions can be derived from two formulae concerning the Laguerre functions: the generating function, equation (24), and the bilinear generating function (frequently called the Hille–Hardy theorem)

$$\sum_{\lambda=0}^{\infty} \frac{\lambda!}{\Gamma(\mu+1+\lambda)} (-h)^\lambda L_\lambda^\mu(x) L_\lambda^\mu(y) = \frac{1}{(xyh)^{\mu/2}} \frac{e^{(x+y)\frac{h}{1+h}}}{1+h} J_\mu \left( 2 \frac{\sqrt{xyh}}{1+h} \right) \quad (29)$$

where  $|h| < 1$ , for arbitrary  $x$  and  $y$ , or  $|h| \leq 1$ , if  $x, y$  are real. This formula gives essentially the completeness of the Laguerre functions. In the limit  $h \rightarrow 1$  the series represents a Dirac function  $\delta(x - y)$  [22, 25]

$$\sum_{\lambda=0}^{\infty} \frac{\lambda!}{\Gamma(\mu+1+\lambda)} \left[ \frac{1}{x^{\mu/2}} e^{-x/2} L_\lambda^\mu(x) \right] \left[ \frac{1}{y^{\mu/2}} e^{-y/2} L_\lambda^\mu(y) \right] = \delta(x - y). \quad (30)$$

All the properties of the two-body Coulomb eigenfunction corresponding to the negative energy spectrum can be studied using these formulae. For positive energies, the Coulomb eigenfunction and its properties have to be derived from a different set of linear

$$\begin{aligned} \Gamma(2\mu+1) \frac{x^{\mu+1/2}}{(1+h)^{2\mu+1}} e^{\frac{x}{2} \frac{h-1}{h+1}} \\ = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} h^{-\frac{1}{2}+u-\mu} \Gamma\left(\frac{1}{2}-u+\mu\right) \Gamma\left(\frac{1}{2}+u+\mu\right) M_{u,\mu}(x) du \end{aligned} \quad (31)$$

and bilinear

$$\begin{aligned} \frac{1}{2\pi i} \int_C h^u \frac{\Gamma\left(\frac{1}{2}-u+\mu\right) \Gamma\left(\frac{1}{2}+u+\mu\right)}{[\Gamma(2\mu+1)]^2} M_{u,\mu}(x) M_{u,\mu}(y) du \\ = \frac{\sqrt{hxy}}{1+h} e^{-\frac{x+y}{2} \frac{1-h}{1+h}} J_{2\mu} \left( 2 \frac{\sqrt{xyh}}{1+h} \right) \end{aligned} \quad (32)$$

generating functions. The parameter  $c$  is such that  $c < \text{Re}(\mu) + \frac{1}{2}$  and  $|\arg(h)| < \pi$ . The contour  $C$  in (32) is a path from  $-i\infty$  to  $i\infty$ , separating the poles of the Gamma function  $\Gamma\left(\frac{1}{2}-u+\mu\right)$  from those of  $\Gamma\left(\frac{1}{2}+u+\mu\right)$  and  $|\arg(h)| < \pi$  [26]. The bilinear generating function can be used to define the completeness of the continuum eigenfunctions.

Having two different sets of generating functions for the negative and positive parts of the energy spectra is due to the fact that they are eigenfunctions defined in different intervals of



the same differential equation. Laguerre polynomials are the eigenfunctions in  $(0, \infty)$  of the two-body Coulomb equation. In the interval  $(0, i\infty)$  the eigenfunctions are  $M_{i\beta, m}(ix)$ . Both systems are connected by the analytic continuation of the relative momentum to the complex plane (see [19, 27]). To obtain a complete set of energy eigenfunctions for a hydrogen-like system, it is necessary to combine the discrete with the continuum ones.

A set of basis functions to deal indistinctly with both the positive and the negative energy spectra can be given using the reciprocal transformation formulae introduced by Erdélyi [28]

$$f_c(x) = \int_{-\infty}^{\infty} g_c(\gamma) e^{-ix/2} F\left[\frac{c}{2} + i\gamma, c, ix\right] d\gamma \quad c > 0 \quad (33)$$

where the function  $g_c(\gamma)$  is given by

$$g_c(\gamma) = \frac{1}{2\pi} \frac{\Gamma\left(\frac{c}{2} - i\gamma\right) \Gamma\left(\frac{c}{2} + i\gamma\right)}{[\Gamma(c)]^2} e^{\pi\gamma} \int_0^{\infty} y^{c-1} e^{-iy/2} F\left[\frac{c}{2} + i\gamma, c, iy\right] f_c(y) dy. \quad (34)$$

These equations can be derived from the bilinear generating function, equation (32).

### 3.1. Spherical coordinates

To write (33) and (34) in terms of solutions (4) of the two-body Schrödinger equation in spherical coordinates, we first introduce the definition  $c = 2l + 2$ . Multiplying both sides of equation (33) by  $(ix)^{l+1}$  and introducing the change of function  $\Psi_{\text{char}}(x) = (ix)^{l+1} f_c(x)$  we get

$$\Psi_{\text{char}}(x) = \int_{-\infty}^{\infty} \mathcal{Z}(\gamma) S_{\gamma, l}(x) d\gamma. \quad (35)$$

This enables one to write any sufficiently regular function  $\Psi_{\text{char}}(r)$  in terms of  $S_{\gamma, l}(r)$ .

The functions  $S_{\gamma, l}(r)$  are

$$S_{\gamma, l}(x) = N_{\gamma, l} (ix)^{l+1} e^{-ix/2} F[l + 1 + i\gamma, 2l + 2, ix] = N_{\gamma, l} M_{-i\gamma, l+1/2}(ix) \quad (36)$$

where  $N_{\gamma, l}$  defines a normalization factor

$$N_{\gamma, l} = \frac{|\Gamma(l + 1 + i\gamma)|}{(i)^{l+1} \Gamma(2l + 2) \sqrt{2\pi}} e^{\frac{\pi}{2}\gamma}. \quad (37)$$

The transformed function  $\mathcal{Z}(\gamma)$  is

$$\mathcal{Z}(\gamma) = \int_0^{\infty} S_{\gamma, l}(y) \frac{1}{y} \Psi_{\text{char}}(y) dy. \quad (38)$$

The connection between the Whittaker function  $M_{\sigma, m}(x)$ , and the bilinear generating function (32) is evident from the preceding equations. This kind of integral representation has been used by Buchholz to write various types of plane waves in different coordinate systems, see [22].

An orthogonality relation for the  $S_{\gamma, l}(x)$  functions can be established by setting  $\Psi_{\text{char}}(x) = S_{\gamma', l}(x)$  in equations (35) and (38), to obtain

$$\int_0^{\infty} S_{\gamma', l}(y) \frac{1}{y} S_{\gamma, l}(y) dy = \delta(\gamma' - \gamma). \quad (39)$$

One sees that the weight function is a Coulomb potential with unitary charge. This means that the charge Sturmians are orthogonal with respect to the Coulomb potential. The closure relation is

$$\int_0^{\infty} dy \Psi_{\text{char}}(y) \frac{1}{y} \int_{-\infty}^{\infty} S_{\gamma, l}(x) S_{\gamma, l}(y) d\gamma = \Psi_{\text{char}}(x) \quad (40)$$

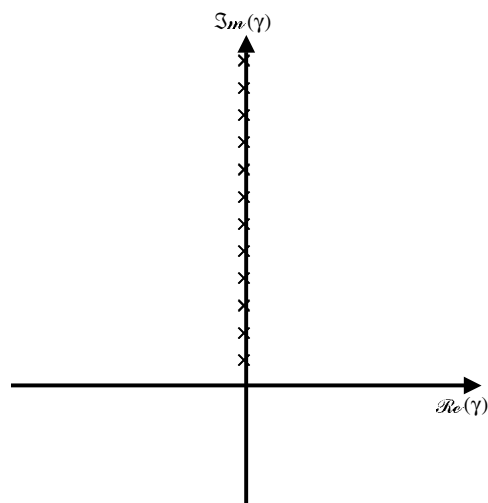


Figure 1. The poles of the Gamma function appearing in the integral of equation (42).

by taking the limit  $h \rightarrow 1$  in equation (32), we get

$$\frac{1}{y} \int_{-\infty}^{\infty} S_{\gamma,l}(x) S_{\gamma,l}(y) d\gamma = \delta(y - x). \quad (41)$$

Equations (39) and (40) show that the functions  $S_{\gamma,l}(x)$  form a complete basis set of orthogonal functions.

It is easy to see the relation between these Sturmians and those used before in the literature [3, 6, 13]. For example, to obtain the Ovchinnikov and Macek version of the charge Sturmians [6], we introduce the change of variables  $x = 2kr$  and function  $\tilde{\mathcal{Z}}(\gamma) = \mathcal{Z}(\gamma)/N_{\gamma,l}$  to get

$$\begin{aligned} \tilde{\Psi}_{\text{char}}(r) = & \int_{-\infty}^{\infty} \tilde{\mathcal{Z}}(\gamma) \frac{(2k)^{l+1} \Gamma(l+1+i\gamma) \Gamma(l+1-i\gamma)}{2\pi [\Gamma(2l+2)]^2} e^{\pi\gamma} (2ikr)^{l+1} e^{-ikr} \\ & \times F[l+1+i\gamma, 2l+2, 2ikr] d\gamma. \end{aligned} \quad (42)$$

We require that the function  $\tilde{\mathcal{Z}}(\gamma)$  does not have poles on the upper half-plane in the  $\gamma$  space, which includes the whole real axis. Then the only poles of the integrand of equation (42) in the upper plane are those of the Gamma function  $\Gamma(l+1+i\gamma)$ , see figure 1. According to the conditions under which the Erdélyi reciprocal transformations were established [26], the integral can be evaluated by the residues theorem by closing the contour in the upper plane and including all the poles of the Gamma function  $\Gamma(l+1+i\gamma)$  occurring over the positive imaginary axis at  $\gamma = i(l+1+n)$ . We finally obtain

$$\tilde{\Psi}_{\text{char}}(r) = \sum_{n=l+1}^{\infty} A_n S_{n,l}^{OM}(r) \quad (43)$$

where the coefficients of the series expansion are

$$A_n = i \int_0^{\infty} S_{n,l}^{OM}(y) \frac{1}{y} \tilde{\Psi}_{\text{char}}(y) dy. \quad (44)$$

We define the function  $S_{n,l}^{OM}(r)$  as

$$S_{n,l}^{OM}(r) = \frac{1}{\Gamma(2l+2)} \sqrt{\frac{\Gamma(l+1+n)}{\Gamma(n-l)}} (2ikr)^{l+1} e^{-ikr} F[l+1-n, 2l+2, 2ikr] \quad (45)$$

for  $n = l + 1, l + 2, \dots$ . These functions are proportional to the Sturmian functions defined by Ovchinnikov, with a complex and discrete eigenvalue [6]. The result obtained is a direct consequence of the Hille–Hardy theorem: the discrete series given by (29) can be derived from the bilinear generating function (32).

### 3.2. Parabolic coordinates

To obtain the charge Sturmians in parabolic coordinates, we first replace the charge  $Z$  by  $(\gamma_1 + \gamma_2)Z$  where  $\gamma_1 Z$  and  $\gamma_2 Z$  define the eigenvalues. Then, using the same method of section 2.2, we get

$$S_{\gamma_1, m}(\xi) = N_{\gamma_1, m} M_{-i\gamma_1, m/2}(ik\xi) \quad S_{\gamma_2, m}(\eta) = N_{\gamma_2, m} M_{-i\gamma_2, m/2}(ik\eta) \quad (46)$$

where  $N_{\gamma_i, m}$  are normalization factors, equation (37), with  $l + 1$  replaced by  $(m + 1)/2$ .

We can now analyse the boundary conditions of the solutions. For brevity, we restrict our attention to  $S_{\gamma_2, m}(\eta)$ ; a similar analysis can be performed for the function in  $\xi$ . The asymptotic behaviour of  $S_{\gamma_2, m}(\eta)$  at  $\eta \rightarrow \infty$  is obtained from the Whittaker function  $M_{a, c/2}(z)$  (see [22])

$$M_{a, c/2}(z) \xrightarrow{|z| \rightarrow \infty} z^{c/2+1/2} e^{-z/2} \left[ \frac{\Gamma(c+1)}{\Gamma(\frac{c+1}{2} + a)} (-z)^{-c/2-1/2+a} + \frac{\Gamma(c+1)}{\Gamma(\frac{c+1}{2} - a)} z^{-c/2-1/2-a} e^z \right]. \quad (47)$$

With this equation we get

$$S_{\gamma_2, m}(\eta) \xrightarrow{|\eta| \rightarrow \infty} \frac{\Gamma(m+1)}{\Gamma(\frac{1+m}{2} - i\gamma_2) i^{\frac{m+1}{2}}} \tilde{N}_{\gamma_2, m} [(-\eta)^{-i\gamma_2} e^{-i(\eta/2 + \frac{\pi}{4}(m+1))} + (\eta)^{i\gamma_2} e^{i(\eta/2 + \frac{\pi}{4}(m+1))}]. \quad (48)$$

Now we use the normalization factors introduced in equation (46) to get

$$S_{\gamma_2, m}(i\eta) \xrightarrow{|\eta| \rightarrow \infty} \frac{1}{i^{m+1}} [e^{-i(\frac{\eta}{2} + \sigma + \gamma_2 \ln \eta + \frac{\pi}{4}(m+1))} + e^{i(\frac{\eta}{2} + \sigma + \gamma_2 \ln \eta + \frac{\pi}{4}(m+1))}]. \quad (49)$$

One sees that the function  $S_{\gamma_2, m}$  is bounded. Then, the complete solution of the Schrödinger equation in parabolic coordinates reads

$$\Phi = N_{\gamma_1, m} N_{\gamma_2, m} e^{im\phi} \frac{1}{\sqrt{\xi\eta}} M_{-i\gamma_1, m/2}(ik\xi) M_{-i\gamma_2, m/2}(ik\eta).$$

One can obtain the same function but using the theory of generating functions. As before, we show the procedure for the  $\eta$  function, the analysis for the  $\xi$  functions is completely analogous. We write the inverse transformation formulae given by equations (33) and (34) in terms of the solutions of the two-body Coulomb wavefunctions in parabolic coordinates. We first introduce the definition  $c = m + 1$  and replace the variable  $x$  by  $\eta$ . Then, we multiply both sides by  $(i\eta)^{\frac{m+1}{2}}$  and introduce the change of function  $\Psi_{\text{char}}(\eta) = (i\eta)^{\frac{m+1}{2}} f_c(\eta)$ , finally obtaining

$$\Psi_{\text{char}}(\eta) = \int_{-\infty}^{\infty} \mathcal{Z}(\gamma) S_{\gamma_2, l}(\eta) d\gamma \quad (50)$$

where the parabolic Sturmian function  $S_{\gamma, l}(\eta)$  is defined by (46). The transformed function  $\mathcal{Z}(\gamma)$  is

$$\mathcal{Z}(\gamma) = \int_0^{\infty} S_{\gamma_2, l}(\eta) \frac{1}{\eta} \Psi_{\text{char}}(\eta) d\eta \quad (51)$$

and the orthogonality and closure relations follow

$$\int_0^{\infty} S_{\gamma_2, l}(\eta) \frac{1}{\eta} S_{\gamma_2', l}(\eta) d\eta = \delta(\gamma - \gamma') \quad (52)$$

$$\int_{-\infty}^{\infty} S_{\gamma_2, l}(\eta') S_{\gamma_2, l}(\eta) d\gamma = \delta(\eta - \eta'). \quad (53)$$

Equations (50)–(53) allow one to represent any sufficiently regular function  $\Psi_{\text{char}}(\eta)$  in terms of the charge parabolic Coulomb Sturmian  $S_{\gamma_2, l}$ .

Using the method given in the preceding section, we can derive a set of Sturmian functions in parabolic coordinates similar to those introduced by Ovchinnikov in spherical coordinates. We first rewrite the inverse transformations defined by equations (50) and (51) as follows:

$$\begin{aligned} \tilde{\Psi}_{\text{char}}(\eta) = & \int_{-\infty}^{\infty} \tilde{\mathcal{Z}}(\gamma) \frac{\Gamma\left(\frac{m}{2} + \frac{1}{2} + i\gamma\right) \Gamma\left(\frac{m}{2} + \frac{1}{2} - i\gamma\right)}{2\pi\Gamma(m+1)} e^{\pi\gamma} (\eta)^{\frac{m+1}{2}} \\ & \times e^{-i\eta/2} F\left[\frac{m}{2} + \frac{1}{2} + i\gamma, 1+m, i\eta\right] d\gamma \end{aligned} \quad (54)$$

where  $\tilde{\mathcal{Z}} = \mathcal{Z}\Gamma(m+1)N_{\gamma, m}$ . Now, assuming that the function  $\tilde{\mathcal{Z}}(\gamma)$  does not have poles in the upper plane of  $\gamma$ , the integral can be evaluated by the residues theorem by closing the contour in the upper plane and counting the poles of the Gamma function  $\Gamma\left(\frac{m}{2} + \frac{1}{2} + i\gamma\right)$  at  $\gamma = i\left(\frac{m}{2} + \frac{1}{2} + n\right)$ . This leads to

$$\tilde{\Psi}_{\text{char}}(\eta) = \sum_{n=0}^{\infty} B_n S_{n, m}(\eta) \quad (55)$$

with

$$S_{n, m}(\eta) = \frac{1}{\Gamma(m+1)} \sqrt{\frac{\Gamma(m+1+n)}{\Gamma(n+1)}} (i\eta)^{\frac{m+1}{2}} e^{-i\eta/2} F[-n, 1+m, i\eta] \quad n = 0, 1, 2, \dots \quad (56)$$

and the coefficient  $B_n$  is given by

$$B_n = i \int_0^{\infty} S_{n, m}(y) \frac{1}{y} \tilde{\Psi}_{\text{char}}(y) dy. \quad (57)$$

The functions  $S_{n, m}(\eta)$  are the Sturmian functions, used by Swainson and Drake [25] to write the Coulomb Green function in parabolic coordinates.

The physical applications of the charge Sturmian studied in section 3 are exactly the same as those of the discrete basis developed by different authors (see [1] and references therein). The main contribution of this section is to show that the Sturmian eigenvalues belong to continuum spectra and also to establish the connection with those belonging to discrete spectra developed by other authors.

#### 4. Angular momentum Sturmians

In the preceding sections we showed that any sufficiently regular function can be written as a linear combination (a series and an integral) of energy or charge eigenfunction. Here, we introduce a third kind of representation, that will allow one to write an arbitrary function as a linear combination (an integral) of *angular momentum Sturmian functions* where the integration variable will be the parameter associated with the angular momentum  $l$  or  $m$ . In this case the momentum (or energy) and the charge remain as constants.

The angular momentum Sturmians can be obtained from a general transformation introduced by Wimp [29]

$$f(x) = -\frac{1}{i\pi} \int_0^{\infty} t e^{-i\pi v} \{e^{\pi t} \Lambda(xe^{i\pi} |v + it, v - it) - e^{-\pi t} \Lambda(xe^{i\pi} |v - it, v + it)\} g(t) dt \quad (58)$$

where

$$g(t) = \int_0^\infty \Omega(y|1 - \nu + ix, 1 - \nu - ix) f(y) dy. \quad (59)$$

The functions  $\Lambda(z|\alpha, \beta)$  and  $\Omega(z|\alpha, \beta)$  are defined in terms of the Meijer G-function (see [28], vol I, and also [30]) as follows:

$$\Lambda(z|\alpha, \beta) = G_{p+2,q}^{q-m,p-n+1} \left( z \left| \begin{array}{c} -a_{n+1}, -a_{n+2}, \dots, a_p, \alpha, -a_1, -a_2, \dots, a_n, \beta \\ -b_{m+1}, -b_{m+2}, \dots, b_q, -b_1, -b_2, \dots, b_m \end{array} \right. \right) \quad (60)$$

$$\Omega(z|\alpha, \beta) = G_{p+2,q}^{m,n+2} \left( z \left| \begin{array}{c} \alpha, \beta, a_p \\ b_q \end{array} \right. \right). \quad (61)$$

Since 1983, Yakubovich has been working on these topics and derived more compact expressions for the sort of transformations involving only one Meijer G-function both in the transform and its inverse [31]. This author also discussed in detail the conditions under which the transformation holds.

To obtain the angular momentum Sturmians, we need only consider  $n = p = 0$  and  $m = q = 1$  in (58) and (59). Then,  $\Lambda(z|\alpha, \beta)$  and  $\Omega(z|\alpha, \beta)$  reduce to Whittaker's functions leading to the formula [29]

$$\Psi_{\text{ams}}(z) = -\frac{1}{2\pi} \int_0^{i\infty} \Gamma\left(\frac{1}{2} + i\beta + \frac{\nu}{2}\right) \Gamma\left(\frac{1}{2} + i\beta - \frac{\nu}{2}\right) \nu \sin(\pi\nu) \bar{\mathcal{L}}(\nu) W_{-i\beta, \frac{\nu}{2}}(z) d\nu \quad (62)$$

where the transform function  $\bar{\mathcal{L}}(\nu)$  is given by

$$\bar{\mathcal{L}}(\nu) = \frac{1}{2\pi i} \int_0^\infty \Psi_{\text{ams}}(y) \frac{1}{y^2} W_{-i\beta, \frac{\nu}{2}}(y) dy. \quad (63)$$

The conditions under which formulae (62) and (63) are reciprocal have been studied by Yakubovich and co-workers [32, 33, 37]. One sees that  $W_{-i\beta, \frac{\nu}{2}}(z)$  constitutes a set of doubly orthogonal functions, with orthogonality and closure relations given by

$$\begin{aligned} -\frac{1}{2\pi} \Gamma\left(\frac{1}{2} + i\beta + \frac{\nu}{2}\right) \Gamma\left(\frac{1}{2} + i\beta - \frac{\nu}{2}\right) \nu \sin(\pi\nu) \int_0^\infty W_{-i\beta, \frac{\nu'}{2}}(y) \frac{1}{y^2} W_{-i\beta, \frac{\nu}{2}}(y) dy \\ = 2\pi i \delta(\nu - \nu') \end{aligned} \quad (64)$$

$$\begin{aligned} -\frac{1}{2\pi} \frac{1}{y^2} \int_0^{i\infty} \Gamma\left(\frac{1}{2} + i\beta + \frac{\nu}{2}\right) \Gamma\left(\frac{1}{2} + i\beta - \frac{\nu}{2}\right) \nu \sin(\pi\nu) W_{-i\beta, \frac{\nu'}{2}}(y) W_{-i\beta, \frac{\nu}{2}}(z) d\nu \\ = 2\pi i \delta(y - z). \end{aligned} \quad (65)$$

Following a procedure similar to that of [35], the analytic continuation of the argument  $z$  can be performed on (62) and (63), leading to the set of formulae

$$\Psi_{\text{ams}}(z) = -\frac{1}{2\pi} \int_0^{i\infty} \Gamma\left(\frac{1}{2} + i\beta + \frac{\nu}{2}\right) \Gamma\left(\frac{1}{2} + i\beta - \frac{\nu}{2}\right) \nu \sin(\pi\nu) \bar{\mathcal{L}}(\nu) W_{-i\beta, \frac{\nu}{2}}(iz) d\nu \quad (66)$$

$$\bar{\mathcal{L}}(\nu) = \frac{1}{2\pi i} \int_0^\infty \Psi_{\text{ams}}(y) \frac{1}{y^2} W_{-i\beta, \frac{\nu}{2}}(iy) dy. \quad (67)$$

The function  $W_{-i\beta, \frac{\nu}{2}}(iz)$  satisfies the parabolic Coulomb equation (14) of section 2, where  $\beta$  represents generically the parameter  $\beta_i$  introduced there (the Sommerfeld parameter). Equations (66) and (67) show that it is possible to represent any sufficiently regular function  $\Psi_{\text{ams}}(z)$  as an integral over the parameter corresponding to the angular momentum ( $m$  in this

case). The function  $W_{-i\beta, \frac{\nu}{2}}(iz)$  is irregular at the origin of coordinates and has incoming asymptotic behaviour. An equivalent expression based on the outgoing wavefunction can be equally derived. The irregularity at the origin does not restrict at all the use of the inverse transformation. However, we want to obtain another expression based on the regular Whittaker function  $M_{-i\beta, \frac{\nu}{2}}(iz)$ . To achieve that transformation we rewrite the Whittaker function  $W_{-i\beta, \frac{\nu}{2}}(z)$  in terms of  $M_{-i\beta, \frac{\nu}{2}}(z)$  as follows [22]:

$$W_{-i\beta, \frac{\nu}{2}}(z) = \frac{\pi}{\sin(\pi\nu)} \left[ \frac{M_{-i\beta, -\frac{\nu}{2}}(z)}{\Gamma(\frac{1}{2} + i\beta + \frac{\nu}{2}) \Gamma(1 - \nu)} - \frac{M_{-i\beta, \frac{\nu}{2}}(z)}{\Gamma(\frac{1}{2} - \frac{\nu}{2} + i\beta) \Gamma(1 + \nu)} \right].$$

Substituting this definition in equation (66) for  $F(z)$  we get

$$\begin{aligned} \Psi_{\text{ams}}(z) = & - \left[ \int_0^{i\infty} \bar{\mathcal{L}}(\nu) \frac{\Gamma(\frac{1}{2} + i\beta - \frac{\nu}{2})}{\Gamma(1 - \nu)} M_{-i\beta, -\frac{\nu}{2}}(iz) \frac{\nu}{2} d\nu \right. \\ & \left. - \int_0^{i\infty} \bar{\mathcal{L}}(\nu) \frac{\Gamma(\frac{1}{2} + i\beta + \frac{\nu}{2})}{\Gamma(1 + \nu)} M_{-i\beta, \frac{\nu}{2}}(iz) \frac{\nu}{2} d\nu \right]. \end{aligned} \quad (68)$$

To reduce this expression to a single integral, we introduce the change of variable  $\nu \rightarrow -\nu$  in the first integral. The relation connecting the Whittaker function with different sign in the second parameter is  $W_{-i\beta, \nu}(y) = W_{-i\beta, -\nu}(y)$ , which implies that  $\bar{\mathcal{L}}(-\nu) = \bar{\mathcal{L}}(\nu)$ . Thus,

$$\begin{aligned} \Psi_{\text{ams}}(\eta) &= \int_{-i\infty}^{i\infty} \bar{\mathcal{L}}(\nu) \frac{\Gamma(\frac{1}{2} + i\beta + \frac{\nu}{2})}{\Gamma(1 + \nu)} M_{-i\beta, \frac{\nu}{2}}(ik\eta) \frac{\nu}{2} d\nu \\ &= \int_{-i\infty}^{i\infty} \bar{\mathcal{L}}(\nu) \varphi_{2,k,\nu}(\eta) \frac{\nu}{2} d\nu \end{aligned} \quad (69)$$

and

$$\begin{aligned} \bar{\mathcal{L}}(\nu) &= \frac{1}{2\pi i} \int_0^{\infty} \frac{1}{y^2} \Psi_{\text{ams}}(y) W_{-i\beta, \frac{\nu}{2}}(iy) dy \\ &= \frac{1}{2\pi i} \int_0^{\infty} \frac{1}{y^2} \Psi_{\text{ams}}(y) \bar{\varphi}_{2,k,m}(y) dy. \end{aligned} \quad (70)$$

In equation (69) the variable  $z$  was replaced by  $z = k\eta$ , connecting the inverse transformation with  $\varphi_{2,k,\nu}(\eta)$  of (14) and (15); it could also be defined as  $z = k\xi$  establishing a connection with  $\varphi_{1,k,\nu}(\xi)$  of (14) and (15). As we can see the integrand of this equation is defined in terms of the solutions of the two-body Coulomb problem in parabolic coordinates.

If the definition of the Whittaker function  $W_{-i\beta, \nu}(iy)$  is replaced in  $\bar{\mathcal{L}}(\nu)$ , the following set of inverse transformations is obtained:

$$\Psi_{\text{ams}}(x) = \frac{1}{2} \int_{-i\infty}^{i\infty} \mathcal{L}(\nu) W_{-i\beta, \frac{\nu}{2}}(ix) \nu d\nu \quad (71)$$

$$\mathcal{L}(\nu) = \frac{1}{2\pi i} \int_0^{\infty} y^{-2} \Psi_{\text{ams}}(y) \frac{\Gamma(\frac{1}{2} + i\beta + \frac{\nu}{2})}{\Gamma(1 + \nu)} M_{-i\beta, \frac{\nu}{2}}(iy) dy. \quad (72)$$

A similar transformation can be defined for the real argument of Whittaker's functions.

Even though the definitions of the functions in  $\Psi_{\text{ams}}(\eta)$  and  $\bar{\mathcal{L}}(\nu)$ ,  $\mathcal{L}(\nu)$  are given in terms of different functions, it is still possible to define closure and orthogonality relations. Substituting the expression for  $\bar{\mathcal{L}}(\nu)$  in (69) we get the closure relation

$$\frac{1}{\eta^2} \int_{-i\infty}^{i\infty} \bar{\varphi}_{2,k,v}(\eta) \varphi_{2,k,v}(\eta') \frac{v}{2} dv = 2\pi i \delta(\eta - \eta'). \quad (73)$$

If we define  $\Psi_{\text{ams}}(\eta) = \varphi_{2,k,v'}(\eta)$  then, from equations (69) and (70) we find the orthogonality relation

$$\frac{1}{2\pi i} \int_0^\infty \varphi_{2,k,v'}(\eta) \frac{v}{2\eta^2} \bar{\varphi}_{2,k,v}(\eta) d\eta = \delta(v - v'). \quad (74)$$

As we see in this equation, the functions  $\varphi_{2,k,v}(\eta)$  and  $\bar{\varphi}_{2,k,v}(\eta)$  are orthogonal with respect to the potential  $1/\eta^2$  which represents the centrifugal potential in parabolic coordinates. The weight function in the orthogonality relation is associated with the parameter employed as the variable of integration, in the same way as the charge Sturmians.

It is interesting to see that some well-known transformations can be obtained as particular cases of the generalized angular Coulomb representation previously discussed. When the parameter  $\beta_i$  is set to zero in equations (62) and (63) and the relations between the Whittaker and Bessel functions  $K_\nu(z)$  [21] are used, we get the inverse transformation defined by Lebedev in 1946 [34]. This reduction was already mentioned by Wimp in his paper of 1964 [29]. The condition  $\beta_i = 0$  is equivalent to setting the charges of the particles equal to zero. This defines an inverse transformation in terms of the solution of the plane wave Schrödinger equation. Applying the same limit to (69) and (70), and using the relations between the Whittaker  $M_{a,b}(x)$  ( $W_{a,b}(x)$ ) and the Bessel function  $J_n(x)$  ( $H_n^{(2)}(x)$ ) respectively [22], we get the inverse transformation introduced by Kontorovich and Lebedev [35] (see also [38], vol II).

The inverse transformations used by Macek and Ovchinnikov [4] result from the limit and relations just mentioned but applied to equations (71) and (72). If the limit of  $\beta_i = 0$  is applied to the analytic continuation of equations (71) and (72), another Lebedev inverse transformation [4, 36] is obtained. Other Kontorovich–Lebedev inverse transformations can be defined by taking  $\beta_i = 0$  in (66), (67), and in those which result from the analytic continuation of (69), (70). These two cases, to our knowledge, have not been previously discussed in the literature.

It is easy to show that any sufficiently regular function can be represented in terms of Coulomb wavefunctions belonging to the continuous spectra of the energy, where the integration is performed over a generalization of the angular momentum. The expansion of a general function  $\Psi(\xi, \eta, \phi)$  of the variables  $\xi$ ,  $\eta$  and  $\phi$  in terms of generalized angular momentum Sturmian functions is

$$\begin{aligned} \Psi(\xi, \eta, \phi) = & \sum_{m=-\infty}^{\infty} \int_{-i\infty}^{i\infty} \int_{i\infty}^{-i\infty} \bar{\Psi}_m(v_1, v_2) \frac{\Gamma\left(\frac{1+m+v_1}{2} + i\beta_1\right)}{\Gamma\left(\frac{1+m+v_1}{2}\right)} M_{-i\beta_1, \frac{v_1+m}{2}}(ik\xi) \\ & \times \frac{\Gamma\left(\frac{1+m+v_2}{2} - i\beta_2\right)}{\Gamma\left(\frac{1+m+v_2}{2}\right)} M_{-i\beta_2, \frac{v_2+m}{2}}(-ik\eta) v_1 v_2 dv_1 dv_2 \end{aligned} \quad (75)$$

where the transform  $\bar{\Psi}_m(v_1, v_2)$  is obtained by using the inverse transformation in each of the coordinates. Note that the integration contour is moved off the imaginary axes because of the presence of the eigenvalue of the projection of the angular momentum  $L_z$ .

Analogous to the charge Sturmians, the same set of functions is used with the continuous as well as the discrete spectra of the energy. In general, when dealing with problems involving charged particles, it is necessary to properly take into account the long-range tail that it produces in the wavefunction. The angular momentum Sturmians have the advantage, over the charge Sturmians, that all the basis functions have the proper asymptotic form

$$\begin{aligned}
M_{-i\beta, \frac{\nu}{2}}(ikz) &\longrightarrow \frac{\Gamma(1+\nu)}{\Gamma\left(\frac{1+\nu}{2} + i\beta\right)} (ikz)^{i\beta} e^{\frac{ikz}{2}} {}_2F_0\left[\frac{1+\nu}{2} + i\beta, \frac{1-\nu}{2} + i\beta; ; 1/(ikz)\right] \\
&\quad + \frac{\Gamma(1+\nu)}{\Gamma\left(\frac{1+\nu}{2} - i\beta\right)} (ikz)^{-i\beta} e^{-\frac{ikz}{2}} e^{\pm i\pi(-i\beta - \frac{1+\nu}{2})} \\
&\quad \times {}_2F_0\left[\frac{1+\nu}{2} + i\beta, \frac{1-\nu}{2} + i\beta; ; -1/(ikz)\right] \quad (76) \\
W_{-i\beta, \frac{\nu}{2}}(ikz) &\longrightarrow (ikz)^{-i\beta} e^{-\frac{ikz}{2}} {}_2F_0\left[\frac{1+\nu}{2} + i\beta, \frac{1-\nu}{2} + i\beta; ; -1/(ikz)\right].
\end{aligned}$$

One sees that for large values of the coordinates, the angular momentum Sturmians lead to the correct asymptotic eikonal phase (a distorted plane wave) in each of the coordinates considered. Then, the expansion has to take care only of the behaviour in the internal region where the dynamics is important and the behaviour of the wavefunction departs from the pure Coulomb case. For example, choosing  $\beta_1 = \frac{Z\mu}{k}$  and  $\beta_2 = 0$  in the expansion (75), one obtains a distorted plane wave as an asymptotic form in the coordinate  $\xi$ . A similar set of inverse transformations can be defined with the spherical Coulomb eigenfunctions as the kernel of the transformation, where the integration is performed over a generalization of the angular momentum  $l$ .

The representation for an arbitrary function in terms of the regular and irregular Whittaker functions was obtained using a well-defined integration contour. However, the contour can, and in some cases must be, distorted, moved away from the imaginary axis or even bent, to get the convergence of the integrals. In systems of three particles interacting via zero-range potential, Gasaneo and co-workers used a Kontorovich–Lebedev representation to write the solution of the problem [10]. They found that the integration contour is not just a straight line along the imaginary axes but a combination of contours that lead to a convergent integral representation of a given function. The same procedure was used by Macek and Ovchinnikov when dealing with the three-body Coulomb problem [4]. In both cases, the coefficient of the expansions was obtained as the solution of a three-term recurrence relation and no inverse transformation was necessary. A similar procedure is expected to be useful when dealing with the Coulomb wavefunction representations based on the fact that these functions satisfy recurrence relations similar to those of the Bessel functions

$$\left(\beta + \frac{\mu+1}{2}\right) M_{\beta+\frac{1}{2}, \frac{\mu+1}{2}}(z) + M_{\beta+\frac{1}{2}, \frac{\mu-1}{2}}(z) = \frac{\mu}{z^{\frac{1}{2}}} M_{\beta, \frac{\mu}{2}}(z). \quad (77)$$

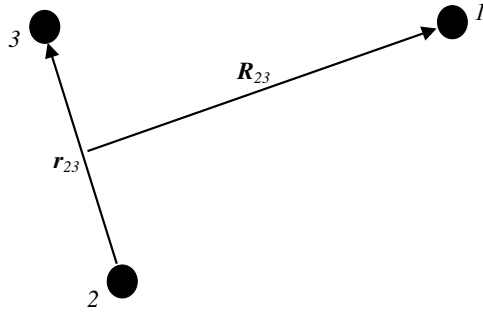
## 5. A proposal for a three-body Coulomb wavefunction

We can make use of the angular Sturmians to obtain a basis representation for the three-body Coulomb problem. Introducing the definitions  $\mu = 0$ ,  $\beta \rightarrow -i\beta + \frac{1}{2}$ ,  $z = ik\eta$  and  $\Psi_{\text{ams}}(z) = z^{\frac{\mu+1}{2}} \Psi(z)$  in equation (27), the following representation for a sufficiently regular function  $\Psi_{\text{ams}}(z)$  results:

$$\Psi_{\text{ams}}(z) = \sum_{s=0}^{\infty} a_s M_{\beta, s}(ik\eta). \quad (78)$$

Equation (78) shows that the function  $\Psi_{\text{ams}}(\eta)$  can be expanded in terms of angular momentum Coulomb Sturmian  $M_{\beta, s}(ik\eta)$ . Equation (78) is the one-dimensional version of the basis used by Gasaneo and co-workers to represent the  $\Phi_2$  model for three charged particles [14, 15]. This is also the basis discussed by Gasaneo [16] and also by Miraglia *et al* [17].





**Figure 2.** One of the three Jacobi pairs that can be used to study a three-body system.

To deal with the six-dimensional three-body Coulomb problem, we use the set of generalized parabolic coordinates defined by Klar [39]:

$$\begin{aligned} \xi_1 &= r_{23} + \widehat{\mathbf{k}}_{23} \cdot \mathbf{r}_{23} & \xi_2 &= r_{13} + \widehat{\mathbf{k}}_{13} \cdot \mathbf{r}_{13} & \xi_3 &= r_{12} + \widehat{\mathbf{k}}_{12} \cdot \mathbf{r}_{12} \\ \eta_1 &= r_{23} - \widehat{\mathbf{k}}_{23} \cdot \mathbf{r}_{23} & \eta_2 &= r_{13} - \widehat{\mathbf{k}}_{13} \cdot \mathbf{r}_{13} & \eta_3 &= r_{12} - \widehat{\mathbf{k}}_{12} \cdot \mathbf{r}_{12} \end{aligned} \quad (79)$$

where  $\mathbf{r}_{ij}$  and  $\mathbf{k}_{ij}$ , with  $i, j = 1, 2, 3$  and  $i \neq j$ , are the relative coordinate and momentum vectors between the particles  $i$  and  $j$ . The free particle wavefunction is written in these coordinates as follows:

$$\begin{aligned} \chi_{\mathbf{k}_{23}, \mathbf{K}_{23}}(\mathbf{r}_{23}, \mathbf{R}_{23}) &= \chi_{\mathbf{k}_{23}, \mathbf{K}_{23}}(\xi_1, \eta_1, \xi_2, \eta_2, \xi_3, \eta_3) = e^{i\mathbf{k}_{23} \cdot \mathbf{r}_{23} + i\mathbf{K}_{23} \cdot \mathbf{R}_{23}} \\ &= e^{i\frac{1}{2} \frac{m_2+m_3}{M} k_{23}(\xi_1-\eta_1) + i\frac{1}{2} \frac{m_1+m_3}{M} k_{13}(\xi_2-\eta_2) + i\frac{1}{2} \frac{m_1+m_2}{M} k_{12}(\xi_3-\eta_3)} \end{aligned} \quad (80)$$

where  $m_i$ ,  $i = 1, 2, 3$ , are the masses of each of the particles and  $M = m_1 + m_2 + m_3$ . The vectors  $\mathbf{r}_{23}$  and  $\mathbf{R}_{23}$  form one of the three Jacobi pairs  $\{\mathbf{r}_{ij}, \mathbf{R}_{ij}\}$ , where  $i, j = 1, 2, 3$  with  $i \neq j$ , one of these pairs is shown in figure 2.

The continuum wavefunction for three charged particles is usually written as the product of the plane waves times a function which includes all the dynamics. To write this function in terms of the angular momentum Sturmian functions introduced in the preceding section we need to do some transformations to get the plane wave given by (80). These transformations lead to the following parabolic coordinates representation:

$$\Psi(\mathbf{r}_{23}, \mathbf{R}_{23}) = \chi_{\mathbf{k}_{23}, \mathbf{K}_{23}}(\mathbf{r}_{23}, \mathbf{R}_{23}) \int_{-i\infty}^{i\infty} \tilde{\Psi}(v) \mathcal{F}_1(v_1, v_2, \mathbf{r}_{23}) \mathcal{F}_2(v_3, v_4, \mathbf{r}_{13}) \mathcal{F}_3(v_5, v_6, \xi_3, \mathbf{r}_{12}) dv \quad (81)$$

where  $dv = \prod_{r=1}^6 \frac{v_r}{2} dv_r$  and  $i = 1, 2, 3$  and

$$\begin{aligned} \mathcal{F}_l(v_r, v_s, \mathbf{r}_{mn}) &= \frac{\Gamma(i\alpha_l + v_r)}{\Gamma(1 + 2v_r)} (-i(k_{mn}r_{kl} + \mathbf{k}_{mn} \cdot \mathbf{r}_{mn}))^{v_r} \\ &\quad \times {}_1F_1[i\alpha_l + v_r, 1 + 2v_r, -i(k_{mn}r_{mn} + \mathbf{k}_{mn} \cdot \mathbf{r}_{mn})] \\ &\quad \times \frac{\Gamma(i\beta_l + v_s)}{\Gamma(1 + 2v_s)} (i(k_{mn}r_{mn} - \mathbf{k}_{mn} \cdot \mathbf{r}_{mn}))^{v_s} \\ &\quad \times {}_1F_1[i\beta_l + v_s, 1 + 2v_s, i(k_{mn}r_{mn} - \mathbf{k}_{mn} \cdot \mathbf{r}_{mn})] \end{aligned} \quad (82)$$

with  $l, m, n = 1, 2, 3$  and  $l \neq m \neq n$ . As we can see in the last equation,  $\mathcal{F}_l(v_r, v_s, \mathbf{r}_{mn})$  is defined as a function of  $\mathbf{r}_{mn}$ . Each of the relative vectors  $\mathbf{r}_{mn}$  has to be written as a function of one Jacobi pair  $\{\mathbf{r}_{ij}, \mathbf{R}_{ij}\}$ .

If the function  $\Psi(\mathbf{r}_{23}, \mathbf{R}_{23})$  were known, then the inverse transform  $\tilde{\Psi}(\nu)$  would be defined by

$$\tilde{\Psi}(\nu) = \frac{1}{(2i\pi)^6} \int_0^\infty \Psi(\mathbf{r}_{23}, \mathbf{R}_{23}) \mathcal{W}_1(\nu_1, \nu_2, \mathbf{r}_{23}, \mathbf{R}_{23}) \times \mathcal{W}_2(\nu_3, \nu_4, \mathbf{r}_{23}, \mathbf{R}_{23}) \mathcal{W}_3(\nu_5, \nu_6, \mathbf{r}_{23}, \mathbf{R}_{23}) J \, d\mathbf{r}_{23} \, d\mathbf{R}_{23} \quad (83)$$

where

$$\begin{aligned} \mathcal{W}_l(\nu_r, \nu_s, \mathbf{r}_{23}, \mathbf{R}_{23}) &= (-i(k_{mn}r_{mn} + \mathbf{k}_{mn} \cdot \mathbf{r}_{mn}))^{\nu_r} \\ &\times U[i\alpha_l + \nu_r, 1 + 2\nu_r, -i(k_{mn}r_{mn} + \mathbf{k}_{mn} \cdot \mathbf{r}_{mn})] \\ &\times (i(k_{mn}r_{mn} - \mathbf{k}_{mn} \cdot \mathbf{r}_{mn}))^{\nu_s} \\ &\times U[i\beta_l + \nu_s, 1 + 2\nu_s, i(k_{mn}r_{mn} - \mathbf{k}_{mn} \cdot \mathbf{r}_{mn})]. \end{aligned} \quad (84)$$

$U[a, b, z]$  is the irregular Kummer function (21) The symbol  $J$  involves the parabolic coordinates in the denominator of equation (83) and the Jacobian connecting the parabolic coordinates with the Cartesian in each of the Jacobi pairs. In general the function  $\Psi(\mathbf{r}_{23}, \mathbf{R}_{23})$  is unknown, so the recurrence relation of the Kummer function has to be used to transform the differential equation satisfied by  $\Psi(\mathbf{r}_{23}, \mathbf{R}_{23})$  into a recurrence relation for the coefficient  $\tilde{\Psi}(\nu)$ .

This extension can be performed to any number of coordinates and it is fully justified by the extension given by Yakubovich [33]. The parameters  $\alpha_i$  and  $\beta_i$  (with  $i = 1, 2, 3$ ) must be chosen according to the asymptotic condition. By choosing properly  $\alpha_i$  and  $\beta_i$  the eight different kinds of asymptotic behaviour described by Klar [39] for Redmond's region can be satisfied. As an example we chose  $\alpha_l = \frac{Z_m Z_n \nu_{mn}}{k_{mn}}$ , with  $l, m, n = 1, 2, 3$  and  $l \neq m \neq n$ , and  $\beta_i = 0$  with  $i = 1, 2, 3$ . In this case we get incoming conditions in the  $\Omega_0$  region where the distances between all the particles tend to infinity [39, 40]. This region is defined by the situation  $\hat{\mathbf{r}}_{ij} \approx \hat{\mathbf{k}}_{ij}$ ,  $r_{ij}, R_{ij} \rightarrow \infty$  and  $r_{ij}/R_{ij} \rightarrow \text{constant} \neq 0$ ; the function  $\Psi(\mathbf{r}_{23}, \mathbf{R}_{23})$  in that limit results in

$$\begin{aligned} \Psi(\mathbf{r}_{23}, \mathbf{R}_{23})|_{r_{23}/R_{23} \rightarrow \text{constant}} &\rightarrow \chi_{\mathbf{k}_{23}, \mathbf{K}_{23}}(\mathbf{r}_{23}, \mathbf{R}_{23}) \mathcal{E}_1(\mathbf{r}_{23}, \mathbf{R}_{23}) \\ &\times \mathcal{E}_2(\mathbf{r}_{23}, \mathbf{R}_{23}) \mathcal{E}_3(\mathbf{r}_{23}, \mathbf{R}_{23}) \int_{-\infty}^{\infty} \tilde{\Psi}(\nu) \, d\nu. \end{aligned} \quad (85)$$

Here  $\mathcal{E}_i(\mathbf{r}_{23}, \mathbf{R}_{23})$ , with  $i = 1, 2, 3$ , represents an eikonal phase

$$\mathcal{E}_i(\mathbf{r}_{23}, \mathbf{R}_{23}) = e^{i \frac{Z_m Z_n \nu_{mn}}{k_{mn}} \log(k_{mn}r_{mn} + \mathbf{k}_{mn} \cdot \mathbf{r}_{mn})} \quad (86)$$

with  $l, m, n = 1, 2, 3$  and  $l \neq m \neq n$ . It has been proved by Kim and Zubarev [41] and by Jones and Madison [42] that the so-called C3 wavefunction [43] has the correct asymptotic behaviour in all the regions in the coordinate [40] and momenta space. So, a Sturmian representation of a general three-body Coulomb wavefunction has to have the same limit as the C3 function in the asymptotic regions both in momenta and coordinates. Another important condition to be fulfilled by the angular momentum Sturmian integral representation (81) is that it should be convergent when the different limits on the coordinates are moved inside the integral symbol. For example, the convergence of the integral of  $\tilde{\Psi}(\nu)$  in (85) allows one to move the limit  $r_{ij}, R_{ij} \rightarrow \infty$  and  $r_{ij}/R_{ij} \rightarrow \text{constant} \neq 0$  inside the integral (81).

The integral of  $\tilde{\Psi}(\nu)$  defines the normalization of the wavefunction  $\Psi(\mathbf{r}_{23}, \mathbf{R}_{23})$  as

$$N = 1 \int_{-\infty}^{\infty} \tilde{\Psi}(\nu) \, d\nu. \quad (87)$$

It is worthwhile mentioning that deep into the condensation region where  $r_{ij}, R_{ij} \rightarrow 0$ , the angular Sturmian representation of  $\Psi(\mathbf{r}_{23}, \mathbf{R}_{23})$  reduces to a Mellin–Barnes integral [38] representation

$$\begin{aligned} \Psi(\mathbf{r}_{23}, \mathbf{R}_{23}) &= \chi_{\mathbf{k}_{23}, \mathbf{K}_{23}}(\mathbf{r}_{23}, \mathbf{R}_{23}) \int_{-i\infty}^{i\infty} \tilde{\Psi}(v) \prod_{j=1}^3 \frac{\Gamma(i\alpha_j + v_{2j-1})\Gamma(i\beta_j + v_{2j})}{\Gamma(1 + 2v_{2j-1})\Gamma(1 + 2v_{2j})} \\ &\quad \times (-i(k_{23}r_{23} + \mathbf{k}_{23} \cdot \mathbf{r}_{23}))^{v_1} (i(k_{23}r_{23} - \mathbf{k}_{23} \cdot \mathbf{r}_{23}))^{v_2} \\ &\quad \times (-i(k_{13}r_{13} + \mathbf{k}_{13} \cdot \mathbf{r}_{13}))^{v_3} (i(k_{13}r_{13} - \mathbf{k}_{13} \cdot \mathbf{r}_{13}))^{v_4} \\ &\quad \times (-i(k_{12}r_{12} + \mathbf{k}_{12} \cdot \mathbf{r}_{12}))^{v_5} (i(k_{12}r_{12} - \mathbf{k}_{12} \cdot \mathbf{r}_{12}))^{v_6} dv. \end{aligned} \quad (88)$$

This result is obtained after evaluating the Kummer functions of the integral (81) in the limit  $r_{23}, r_{13}, r_{12} \rightarrow 0$ , which is equivalent to  $r_{ij}, R_{ij} \rightarrow 0$ . A difference of a power series representation, the Mellin–Barnes integral as well as the angular momentum Sturmian representation can take into account the well-known logarithmic term characteristic of the Coulomb potential.

## 6. Conclusions and outlook

In this paper we have considered three alternative integral representations to deal with Coulomb problems. We showed that after the variable separation processes both in spherical and parabolic coordinates the ‘radial’ Schrödinger equation depends upon three parameters: the momentum  $k$ , the charge of the particles and the angular momentum quantum number. The energy eigenfunction results from the process of solving that equation when the momentum is considered the eigenvalue. In terms of these eigenfunctions a sufficiently regular function can be written as its linear combination. The spectrum of the energy has a discrete and a continuum part. The wavefunctions corresponding to the discrete and the continuum parts have been used in the representation, otherwise the set of functions is not complete.

Charge Sturmian functions in spherical coordinates were derived from the theory of generating functions. The corresponding set of basis functions in parabolic coordinates was presented based on the theory of differential equations and also by a generating function procedure. Both sets of functions were essentially introduced by Erdélyi in 1941. It was shown that the charge Sturmian eigenvalue in each of the coordinates gives rise to continuous spectra for the charge running from  $-\infty$  to  $\infty$ . The Sturmian functions derived in spherical coordinates were compared with those previously introduced by other authors. Our functions are those introduced by Szmytkowski. When our Sturmians are used to represent an arbitrary function without poles, the integral can be evaluated by the residues theorem leading to the representation obtained by Ovchinnikov and Macek. The energy  $E$  enters the Sturmian functions as a parameter. This means that once a Sturmian representation of a given function is performed, the energy  $E$  can be freely extended to the complex plane. Under certain conditions, a discrete Sturmian representation can be obtained in agreement with those discussed by Maquet. We showed that our charge Sturmian functions in parabolic coordinates and those introduced by Swainson and Drake [25] are related. When an arbitrary function without poles is written in terms of these Sturmians, those of Swainson and Drake can be obtained by solving the integral by the residues theorem. The orthogonality and closure relations were given for all the cases discussed.

We also introduced the generalized angular momentum Sturmian functions, derived from the theory of non-convolution transformation discussed by Marichev and Yakubovich [30, 33]. A set of inverse transformations with Coulomb wavefunction as kernel was presented.

In this case the angular momentum, the third parameter appearing in the Schrödinger equation, was used as the integration variable. Three representations were introduced, two based on the irregular Coulomb wavefunction and one based on the regular one. The difference between those based on the irregular Whittaker function is given by their inverse transform. One of them gives the inverse transform in terms of an irregular Whittaker function and the second in terms of a regular one. We also presented the inverse transformation which involves the regular and the irregular functions in their representation. Orthogonality and closure relations were also presented for these representations. The connection with different Kontorovich–Lebedev inversion formulae was also discussed. We have also shown that the transformation involving Whittaker functions can be considered as generalizations of all Kontorovich–Lebedev transformations reported in the literature [28, 32]. One can also obtain the angular Sturmian functions from the solution of an eigenvalue problem. That analysis, which will be presented in a separate paper, follows the steps sketched in [44].

As an application to the three-body Coulomb problem, we showed how to represent a six-dimensional function of the generalized parabolic coordinates of Klar in terms of the angular momentum Sturmian functions. We also gave the inverse transformation to be used in the case of representing a known function. The generalization is justified by the generalization to any arbitrary number of dimensions of the index transformation of Yakubovich. We believe that the angular momentum Sturmian basis is the proper one to deal with the three-body Coulomb problem in Klar’s coordinates. By fixing properly the coefficients  $\alpha$  and  $\beta$  Redmond’s asymptotic condition comes out naturally. Besides, the very characteristic logarithmic terms, a signature of the Coulomb interaction, are already included within the basis. This is an issue where the discrete angular Sturmian functions of Gasaneo [16] and Miraglia [17] fail. The discrete basis is equivalent to a power series and it is well known that a power series does not allow us to write the exact solution of a three-body system with long-range interactions. In the representation given here, the integration contour was fixed, but it is possible to bend it to allow the wavefunction to satisfy channel boundary conditions. These topics are right now under investigation. Another interesting property of the angular momentum Sturmian functions is that they satisfy three-term recurrence relations. These relations appear to be very useful while dealing with the Schrödinger equation. This would enable one to transform the Schrödinger equation into a difference equation [4, 45], and a similar procedure can be implemented in Klar’s coordinates and it will lead to a six-dimensional difference equation.

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