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Note

Spherical Coulomb Functions: Recurrence Relations and Continued Fractions

In this note we find continued fractions for the ratios $-(dF_L/d\rho)/F_L$ and $-(dG_L/d\rho)/G_L$, $F_L(\gamma,\rho)$ and $G_L(\gamma,\rho)$ being respectively the regular and the irregular spherical Coulomb functions of Lth order.

1. Introduction

Consider the linear operators h_L^+ and h_L^- [1],

$$h_L^{\pm} = \left(v_L \pm \frac{d}{d\rho}\right)\Big/ q_L^{1/2}, \qquad v_L = \frac{L}{\rho} + \frac{\gamma}{L}, \qquad q_L = 1 + \left(\frac{\gamma}{L}\right)^2, \tag{1.1}$$

defined in the domain $D \equiv (0 < \rho < +\infty, -\infty < \gamma < +\infty)$ for any positive integer: $L = 1, 2,\ldots$. Using (1.1) we can write the radial equations for the spherical Coulomb functions [2],

$$\left[\frac{d^2}{d\rho^2} + 1 - \frac{2\gamma}{\rho} - \frac{L(L+1)}{\rho^2}\right] u_L(\gamma,\rho) = 0, \tag{1.2}$$

also defined in D and for any non-negative order ($L = 0, 1,\ldots$), in two different ways:

$$h_L^- h_L^+ u_L = u_L, \tag{1.3a}$$

$$h_{L+1}^+ h_{L+1}^- u_L = u_L. \tag{1.3b}$$

For $L = 0$ only Eq. (1.3b) exists.

On multiplying on the left (1.3a) by h_L^+ and (1.3b) by h_{L+1}^- and comparing the results with (1.3b) and (1.3a), respectively, one has

$$u_{L+1} = h_{L+1}^- u_L, \qquad u_{L-1} = h_L^+ u_L. \tag{1.4}$$

Multiplying the first Eq. (1.4) by $q_{L+1}^{1/2}$ and the second by $q_L^{1/2}$, and adding these products, one obtains the familiar three-term recurrence formula,

$$q_L^{1/2} u_{L-1} + q_{L+1}^{1/2} u_{L+1} = (v_L + v_{L+1})\, u_L. \tag{1.5}$$

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The $u_L(\gamma, \rho)$ in all the previous equations may be written as

$$u_L(\gamma, \rho) = aF_L(\gamma, \rho) + bG_L(\gamma, \rho), \tag{1.6}$$

where a and b are constants and $F_L(\gamma, \rho)$ and $G_L(\gamma, \rho)$ are, respectively, the regular and the irregular spherical Coulomb functions [2, 3].

Each one of Eqs. (1.2) can be associated with a Riccati equation. Define

$$z_L = d[\log(1/u_L)]/(d\rho) = -\frac{du_L}{d\rho}\Big/u_L. \tag{1.7}$$

Differentiating $z_L(\gamma, \rho)$ with respect to ρ and eliminating the term $(d^2u_L/d\rho^2)/u_L$ between the result so obtained and Eq. (1.2), one has

$$\frac{dz_L}{d\rho} = z_L^2 + 1 - \frac{2\gamma}{\rho} - \frac{L(L+1)}{\rho^2}. \tag{1.8}$$

The general integral of this equation is (we take $a/b = c$ in (1.6))

$$z_L = -(c\,dF_L/d\rho + dG_L/d\rho)/(cF_L + G_L). \tag{1.9}$$

Note that for $\gamma = 0$ the radial waves defined above become the spherical functions of a free wave. Accordingly, we have [2, 4]

$$F_L(0, \rho) = f_L(\rho) = \rho j_L(\rho), \qquad G_L(0, \rho) = g_L(\rho) = \rho n_L(\rho), \tag{1.10}$$

where $j_L(\rho)$ and $n_L(\rho)$ are the spherical Bessel functions.

2. Recurrence Relations for the $z_L(\gamma, \rho)$

Introduce the functions $\omega_L^-(\gamma, \rho)$ and $\omega_L^+(\gamma, \rho)$ as follows:

$$\omega_L^- = v_{L+1} + z_L, \qquad \omega_L^+ = v_L - z_L. \tag{2.1}$$

By addition,

$$\omega_L^- + \omega_L^+ = v_L + v_{L+1} \tag{2.2}$$

and substituting (2.1) into (1.3) (see (1.1) and (1.7)),

$$q_{L+1}^{1/2} u_{L+1} = \omega_L^- u_L, \qquad q_L^{1/2} u_{L-1} = \omega_L^+ u_L. \tag{2.3}$$

If we eliminate ω_L^- and ω_L^+ between Eqs. (2.2) and (2.3), we recover the three-term recurrence formula (1.5). But we can follow another line of thought: on multiplying Eqs. (2.3), with L changed into $L-1$ in the first, by each other, we obtain

$$\omega_{L-1}^- \omega_L^+ = q_L \tag{2.4}$$

or, according to (2.1),

$$z_{L-1} = -v_L + \frac{q_L}{v_L - z_L}, \qquad z_L = v_L - \frac{q_L}{v_L + z_{L-1}}. \tag{2.5}$$

Recurrence relations (2.5) for the z_L's are numerically unstable, in the sense that, if we use them indiscriminately, we can finish up with a final c in the general solution (1.9) different from the original one. But within the context of the continued fractions to which they give rise, Eqs. (2.5) are quite stable, as we shall see in the following section.

3. Continued Fractions

The first of relations (2.5) leads to the forward (increasing L) continued fraction,

$$z_{L-1}^{(f)} = -v_L + \frac{q_L}{v_L + v_{L+1} -} \frac{q_{L+1}}{v_{L+1} + v_{L+2} -} \cdots \frac{q_{L+n-1}}{v_{L+n-1} - z_{L+n-1}^{(f)}}, \tag{3.1a}$$

and the second, to the backward (decreasing L) continued fraction,

$$z_L^{(b)} = v_L - \frac{q_L}{v_L + v_{L-1} -} \frac{q_{L-1}}{v_{L-1} + v_{L-2} -} \cdots \frac{q_{L-n+1}}{v_{L-n+1} + z_{L-n}^{(b)}}, \tag{3.1b}$$

where n is a non-negative integer. In (3.1b), $0 \leqslant n \leqslant L$.

Change L into $-L$ in (3.1b). We have

$$z_{-L}^{(b)} = v_{-L} - \frac{q_{-L}}{v_{-L} + v_{-(L+1)} -} \frac{q_{-(L+1)}}{v_{-(L+1)} + v_{-(L+2)} -} \cdots \frac{q_{-(L+n-1)}}{v_{-(L+n-1)} - z_{-(L+n)}^{(b)}}. \tag{3.1c}$$

The continued fractions (3.1a) and (3.1c) are equivalent, if we identify $z_{-(L+n)}^{(b)}$ with $z_{L+n-1}^{(f)}$ and use property (c) of the Appendix with $c_s = -1$, to reduce (3.1c) to (3.1a). Note that $v_{-L} = -v_L$, $q_{-L} = q_L$ (see (1.1)). Write, then,

$$z_{-L}^{(b)} = z_{L-1}^{(f)}, \qquad z_L = z_L^{(b)}, \tag{3.2}$$

where the second relation is a definition.

So we have managed to transform a forward continued fraction into a backward one by extending the L-field to all negative integers. Evidently, $z_{-(L+1)}$ is a solution of Eq. (1.8).

Now set (see (3.2))

$$z_{-(L+1)} = -\frac{dF_L}{d\rho}\Big/ F_L, \qquad z_L = -\frac{dG_L}{d\rho}\Big/ G_L, \tag{3.3}$$

since, for the functions defined in (3.3), the continued fractions (3.1) are completely stable. In fact, for $L \gg \rho$, the initial convergents of (3.1) and the first terms of the right-hand-side expansions of (3.3) into power series [5] are the same.

For $L = 0$ Eqs. (3.3) lead to the still missing relation between z_0 and z_{-1} (note that for $L = 0$ Eqs. (2.5) are meaningless, except if $\gamma = 0$). Define, then, ϕ and ζ as follows:

$$F_0(\gamma, \rho) = \frac{\sin\phi}{\zeta^{1/2}}, \qquad G_0(\gamma, \rho) = \frac{\cos\phi}{\zeta^{1/2}}. \tag{3.4}$$

Eliminating F_0 and G_0 between the Wronskian for these functions [2, 3] and Eqs. (3.4),

$$d\phi/d\rho = \zeta. \tag{3.5}$$

Also define

$$\xi = \frac{1}{2}\, d(\log\zeta)/(d\rho) = \frac{1}{2}\frac{d\zeta}{d\rho}\Big/\zeta. \tag{3.6}$$

Differentiating the logarithms of the reciprocals of Eqs. (3.4) with respect to ρ, we obtain, from (1.7), (3.5) and (3.6), z_0 and z_{-1} expressed in terms of ξ, ζ and $\tan\phi$. Eliminating $\tan\phi$ between these expressions, we have

$$z_0 = \xi + \frac{\zeta^2}{\xi - z_{-1}}. \tag{3.7a}$$

Noting that v_0 and q_0 were left undefined (see (1.1)), we set

$$v_{\pm 0} = \pm\xi, \qquad q_0 = \zeta^2, \qquad z_0 = v_{+0} - \frac{q_0}{v_{-0} + z_{-1}}. \tag{3.7b}$$

Thus, the distinct continued fractions (3.1) can be reduced now to a single continued fraction,

$$z_L = v_L - \frac{q_L}{v_L + v_{L-1} -}\,\frac{q_{L-1}}{v_{L-1} + v_{L-2} -}\cdots, \tag{3.8}$$

where L is positive, negative or null. Henceforward, the condition $0 \leqslant n \leqslant L$ for Eq. (3.1b) must be dropped.

It remains to determine ζ, independently of F_0 and G_0 (see (3.4)). Write $u_0 = G_0 + iF_0 = \exp(i\phi)/\zeta^{1/2}$. Then, by (3.5) and (3.6),

$$d[\log(1/u_0)]/(d\rho) = \xi - i\zeta. \tag{3.9}$$

But (3.9) is a complex solution of Eq. (1.8) for $L = 0$ (see (1.7)). The real part of this equation is

$$\frac{d\xi}{d\rho} = \xi^2 - \zeta^2 + 1 - \frac{2\gamma}{\rho}; \tag{3.10}$$

the imaginary part is equal to (3.6). Eliminating ξ between Eqs. (3.6) and (3.10),

$$\zeta^2 = 1 - \frac{2\gamma}{\rho} + \zeta^{1/2}\frac{d^2(\zeta^{-1/2})}{d\rho^2}. \tag{3.11}$$

We already know how to solve Eq. (3.11) for large L [6, 7]. The integral of Eq. (3.11) must satisfy the condition

$$\zeta(\gamma, \rho) \xrightarrow[\rho\to\infty]{} 1 - \gamma/\rho \tag{3.12}$$

derived from $\phi(\gamma, \rho) \underset{\rho\to\infty}{\to} \rho - \gamma\log(2\rho) + \arg\Gamma(1 + i\gamma)$ [2, 3] by means of (3.5).

Now consider some aspects of the previous theory when $\gamma = 0$, i.e., the case of spherical functions of a free wave [4].

From (1.10),

$$F_0(0, \rho) = \sin\rho, \qquad G_0(0, \rho) = \cos\rho. \tag{3.13}$$

Squaring and adding Eqs. (3.4) we have, from (3.13), $\zeta \equiv 1$ and, from (3.6), $\xi \equiv 0$. Equations (3.7b) yield, then,

$$v_{\pm 0} = 0, \qquad q_0 = 1, \qquad z_0 = -1/z_{-1}, \tag{3.14}$$

in agreement with Eqs. (2.5) for $L = \gamma = 0$.

Note that $z_0(0, \rho)$ is a solution of the corresponding Riccati equation, Eq. (1.8), if $z_{-1}(0, \rho)$ is also a solution.

Next, from (3.8) we obtain, setting $L = \gamma = 0$,

$$\tan\rho = \frac{\rho}{1-}\,\frac{\rho^2}{3-}\,\frac{\rho^2}{5-}\cdots, \tag{3.15}$$

if property (c) of the Appendix with $c_s = -\rho$ is used.

Equation (3.8) yields, for $L = -1$ and $\gamma = 0$,

$$\cot\rho = \frac{1}{\rho} - \frac{\rho}{3-}\,\frac{\rho^2}{5-}\,\frac{\rho^2}{7-}\cdots, \tag{3.16}$$

again using (c), with $c_s = -\rho$. Evidently, we can derive (3.16) directly from (3.15), noting that $\cot \rho = 1/\tan \rho$.

Continued fractions (3.15) and (3.16) are well known [3] and represent $\tan \rho$ and $\cot \rho$ for any ρ, even at the points where these functions become infinite: the zeros of $\cos \rho$ for $\tan \rho$ and the zeros of $\sin \rho$ for $\cot \rho$.

Similarly, the continued fraction (3.8) diverges at the zeros of $F_L(\gamma, \rho)$ and $G_L(\gamma, \rho)$, according to whether L is either negative or positive (null). At any other point, (3.8) converges, since we can develop the continued fraction up to the term $q_{-L_0}/[v_{-L_0} - z_{-(L_0+1)}]$ (see (3.1c)) and if L_0 is large enough, $z_{-(L+1)}$ may be determined with the precision we like [5].

4. Numerical Applications

Tables I to III show examples of the continued fractions (3.8) with negative and positive L. The columns headed by $A_L^{(n)}$, $B_L^{(n)}$ and A_n, B_n are calculated according to property (b) of the Appendix.

From the Wronskian for F_L and G_L [2, 3] and from (3.3),

$$G_L = 1/(dF_L/d\rho + z_L F_L). \tag{4.1}$$

TABLE I

$\gamma = 20$, $\rho = 10$

L	n	$A_L^{(n)}$	$B_L^{(n)}$	$z_{-(L+1)} = -\dfrac{dF_L}{d\rho}\Big/F_L$
0	17	0.85874370E 14	−0.48634100E 14	−0.17657234E 01
1	16	−0.39393671E 13	0.22236185E 13	−0.17716020E 01
2	15	0.33090835E 12	−0.18555982E 12	−0.17832974E 01

Note. Here $z_{-(L+1)} \simeq z_{-(L+1)}^{(n)}$, $z_{-(L+1)}^{(n)}$ being the convergent of lowest order satisfying the condition $|z_{-(L+1)}^{(n-1)} - z_{-(L+1)}^{(n)}| < 10^{-9}$.

TABLE II

$\gamma = 20$, $\rho = 10$

L	n	$A_L^{(n)}$	$B_L^{(n)}$	$z_L = -\dfrac{dG_L}{d\rho}\Big/G_L$
16	15	0.41023715E 13	0.17450763E 13	0.23508264E 01
17	13	0.96083956E 10	0.39697762E 10	0.24203872E 01
18	12	0.11494972E 10	0.46127766E 09	0.24919854E 01

Note. $z_L \simeq z_L^{(n)}$, where $z_L^{(n)}$ is the convergent of lowest order obeying the condition $z_L^{(n-1)} - z_L^{(n)} < 10^{-9}$. Note that $n \leqslant L-1$, since $v_{\pm 0}$ and q_0 (see (3.7b)) have not been calculated for $\gamma \neq 0$.

G_L is then determined since we know how to calculate F_L and $dF_L/d\rho$ [5], as well as z_L; (2.3) and (1.5) may now be used in a forward recurrence procedure. Note, however, that a low order G_L always requires solving Eq. (3.11) for ζ (see Table II), which is not dealt with in this work. A few examples of the calculation of F_L, $dF_L/d\rho$, G_L and $dG_L/d\rho$ are shown in Table IV.

TABLE III

Determination of $z_7(0, 10) = -((dg_7/d\rho)/g_7)_{\rho=10}$

n	A_n	B_n	$z_7^{(n)}(0, 10) - v_7(0, 10)$
1	−0.10000000*E* 01	0.13000000*E* 01	−0.76923077*E* 00
2	−0.11000000*E* 01	0.43000000*E* 00	−0.25581395*E* 01
3	0.10000000*E* −01	−0.91300000*E* 00	−0.10952903*E* −01
...	...	...	...
26	−0.35242081*E* 04	0.14283532*E* 04	−0.24673226*E* 01
27	0.12702792*E* 05	−0.51484120*E* 04	−0.24673224*E* 01
28	−0.48557241*E* 05	0.19680136*E* 05	−0.24673224*E* 01
...	...	...	...

Note. In this case $v_{\pm 0} = 0$, $q_0 = 1$ (see (3.14)).

TABLE IV

$\gamma = 20$, $\rho = 10$

L	F_L	$dF_L/d\rho$	G_L	$dG_L/d\rho$
16	0.14629595*E* −15	0.35599119*E* −15	0.14287601*E* 16	−0.33587669*E* 16
17	0.41983684*E* −16	0.10512308*E* −15	0.48369967*E* 16	−0.11707405*E* 17
18	0.11436679*E* −16	0.29465746*E* −16	0.17251557*E* 17	−0.42990628*E* 17

Note. The columns headed by F_L and $dF_L/d\rho$ are calculated as in Ref. [5]. Since the z_L's have been determined already (Table II), the G_L's can be now obtained from Eq. (4.1) and the $dG_L/d\rho$'s, from $dG_L/d\rho = -z_L G_L$ (see (3.3)).

TABLE V

Determination of $z_1(0, \pi/2) - v_1(0, \pi/2)$

n	A_n	B_n	$z_1^{(n)}(0, \pi/2) - v_1(0, \pi/2)$
1	−0.10000000*E* 01	0.63661977*E* 00	−0.15707963*E* 01
2	0.63661977*E* 00	−0.14052847*E* 01	−0.45301835*E* 00
...	...	...	...
9	−0.15829713*E* −05	0.59408697*E* 05	−0.26645448*E* −10
10	0.13128039*E* −06	−0.63665032*E* 06	−0.20620486*E* −12
...	...	...	...

Note. The function $z_0(0, \rho) = \cot \rho$ becomes infinite for $\rho = \pi/2$. Accordingly, by (2.5), $\lim_{n\to\infty} z_1^{(n)}(0, \pi/2) - 2/\pi = 0$. Note that $v_1(0, \pi/2) = 2/\pi$.

Continued fraction (3.8) may be used for the determination of the zeros of $F_L(\gamma, \rho)$ and $G_L(\gamma, \rho)$. Table V illustrates the simplc case of $\pi/2$, zero of $\cos \rho$.

All the calculations were performed an Coimbra University's SIGMA 5 XEROX computer using double-precision FORTRAN-IV programmes.

Appendix

Let [3, p. 19]

$$f = b_0 + \frac{a_1}{b_1+} \frac{a_2}{b_2+} \cdots \frac{a_n}{b_n+} \cdots; \tag{a}$$

the nth convergent of f (b_0 plus the first n fractions in (a)) is given by $f_n = A_n/B_n$, where

$$\begin{aligned} A_n &= b_n A_{n-1} + a_n A_{n-2}; \qquad & B_n &= b_n B_{n-1} + a_n B_{n-2}; \\ A_0 &= b_0, \quad A_{-1} = 1; & B_0 &= 1, \quad B_{-1} = 0. \end{aligned} \tag{b}$$

If $\{c_s\}$ is a set of non-vanishing elements,

$$f_n = b_0 + \frac{c_1 a_1}{c_1 b_1+} \frac{c_1 c_2 a_2}{c_2 b_2+} \cdots \frac{c_{n-1} c_n a_n}{c_n b_n}. \tag{c}$$

The developments (a) and (c) are said to be equivalent.

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