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Note

Determination of Large-Order Spherical Coulomb Functions with an Argument Lying between the Origin and the Common Point of Inflection

1. Fundamental Equations

The spherical Coulomb functions satisfy the radial equation (see Ref. [1])

$$\left[\frac{d^2}{d\rho^2} + \left(1 - \frac{2\gamma}{\rho} - \frac{L(L+1)}{\rho^2}\right)\right] u_L(\gamma, \rho) = 0. \tag{1.1}$$

They are defined in the domain $0 < \rho < +\infty$, $-\infty < \gamma < +\infty$ for any non-negative integer order: $L = 0, 1, \ldots$.

Write, in the neighbourhood of the origin,

$$u_L = c_\sigma \rho^\sigma \exp(\alpha_\sigma), \tag{1.2}$$

c_σ being independent of ρ, and introduce (1.2) into Eq. (1.1). One has

$$\left(\frac{d\alpha_\sigma}{d\rho}\right)^2 + \frac{d^2\alpha_\sigma}{d\rho^2} + \frac{2\sigma}{\rho}\frac{d\alpha_\sigma}{d\rho} + 1 - \frac{2\gamma}{\rho} = 0 \tag{1.3}$$

if σ is one of the roots of the indicial equation for (1.1),

$$\sigma^2 - \sigma - L(L+1) = 0,$$

i.e.,

$$\sigma_1 = L + 1, \qquad \sigma_2 = -L. \tag{1.4}$$

Thus,

$$F_L(\gamma, \rho) = c_{\sigma_1}\rho^{\sigma_1} \exp(\alpha_{\sigma_1}), \qquad G_L(\gamma, \rho) = c_{\sigma_2}\rho^{\sigma_2} \exp(\alpha_{\sigma_2}), \tag{1.5a}$$

where, according to the usual notation, $F_L(\gamma, \rho)$ and $G_L(\gamma, \rho)$ are respectively the regular and the irregular spherical Coulomb functions of order L.

When $\rho \to 0$, or $L \to \infty$, i.e., when $|(2\sigma)/\rho| \gg 1$, we can neglect $(d\alpha_\sigma/d\rho)^2$ in (1.3) and obtain the approximate solution

$$\frac{d\alpha_\sigma}{d\rho} \simeq \frac{\gamma}{\sigma} - \frac{\rho}{2\sigma + 1}. \tag{1.6}$$

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Thus, considering (1.4), (1.5a) and (1.6),

$$F_L(\gamma, \rho) \xrightarrow[\rho\to 0]{} c_{\sigma_1}\rho^{L+1}\left[1 + \frac{\gamma}{L+1}\rho + \cdots\right], \tag{1.7a}$$

$$G_L(\gamma, \rho) \xrightarrow[\rho\to 0]{} c_{\sigma_2}\left(\frac{1}{\rho}\right)^L \times \begin{cases} [1 + 2\gamma\rho \log \rho + \cdots], & L = 0, \\ \left[1 - \frac{\gamma}{L}\rho + \cdots\right], & L \neq 0. \end{cases} \tag{1.7b}$$

The limit for $G_0(\gamma, \rho)$ is obtained directly from (1.3) by putting $\sigma = \sigma_2 = 0$.

The limits (1.7) show (see Refs. [1], [2]) that the coefficients c_{σ_1} and c_{σ_2} are given by

$$c_{\sigma_1} = \frac{\prod_{s=1}^{L}(1 + \gamma^2/s^2)^{1/2}}{(2L+1)!!} \times \left(\frac{2\pi\gamma}{\rho^{2\pi\gamma} - 1}\right)^{1/2}, \qquad c_{\sigma_2} = \frac{1}{(2L+1)\, c_{\sigma_1}}. \tag{1.5b}$$

The finite product in c_{σ_1} is taken equal to 1 for $L = 0$.

A better approximation $d\alpha_\sigma^0/d\rho$ to $d\alpha_\sigma/d\rho$ can now be found. By differentiation of (1.6) with respect to ρ, one has

$$\frac{d^2\alpha_\sigma}{d\rho^2} \simeq \left(\frac{d\alpha_\sigma}{d\rho} - \frac{\gamma}{\sigma}\right)\Big/\rho. \tag{1.8}$$

and, eliminating $d^2\alpha_\sigma/d\rho^2$ between (1.3) and (1.8),

$$\left(\frac{d\alpha_\sigma^0}{d\rho}\right)^2 + \frac{2\sigma+1}{\rho}\frac{d\alpha_\sigma^0}{d\rho} + 1 - \frac{\gamma}{\rho}\frac{2\sigma+1}{\sigma} = 0. \tag{1.9}$$

The solution of Eq. (1.9) we are interested in, is, evidently, the one which goes into (1.6) when $L \to \infty$ (or $\rho \to 0$):

$$\frac{d\alpha_\sigma^0}{d\rho} = -\frac{\sigma + \frac{1}{2}}{\rho} \times \left\{1 - \left[1 + \frac{2\gamma}{\sigma}\frac{\rho}{\sigma + \frac{1}{2}} - \left(\frac{\rho}{\sigma + \frac{1}{2}}\right)^2\right]^{1/2}\right\}. \tag{1.10}$$

The forms (1.5) for $F_L(\gamma, \rho)$ and $G_L(\gamma, \rho)$ are valid in an interval to the right of the origin where these functions are both positive or, what is the same thing, where α_{σ_i}, $i = 1, 2$ and their derivatives are real functions of ρ. We find from (1.10) that such an interval is given for σ_i, $i = 1, 2$, by

$$0 < \rho < \rho_i, \quad \rho_i = (\sigma_i + \tfrac{1}{2}) \times \{\gamma/\sigma_i + (-1)^{i+1}[(\gamma/\sigma_i)^2 + 1]^{1/2}\}, \quad i = 1, 2. \tag{1.11}$$

The ρ_i, $i = 1, 2$ are close to the common point of inflection of $F_L(\gamma, \rho)$ and $G_L(\gamma, \rho)$ (see Eq. (1.1)):

$$\rho_0 = \gamma + [\gamma^2 + L(L+1)]^{1/2} \tag{1.12}$$

(all the other inflection points of these functions coincide with the zeros of $F_L(\gamma, \rho)$ and $G_L(\gamma, \rho)$, which interlace according to a well-known theorem).

Eqs. (1.11) and (1.12) imply

$$\rho_2 < \rho_0 < \rho_1 \,. \tag{1.13}$$

Also, when $L \to \infty$, $\rho_1 = \rho_2 = \rho_0 \to \infty$.

Obviously, the approximation (1.10) to $d\alpha_\sigma/d\rho$ is good only for values of ρ away from ρ_0. This does not matter in the calculations that will follow, since they are performed for values of ρ smaller than ρ_0.

Now we shall obtain solutions in series for α_σ and $d\alpha_\sigma/d\rho$. Let

$$\frac{d\alpha_\sigma}{d\rho} = \sum_{n=1}^{\infty} a_n \rho^n. \tag{1.14}$$

Substitute (1.14) into Eq. (1.3) and equate to zero the algebric sums of the $\{a_n\}$ belonging to the same ρ^n. One has

$$a_0 = \gamma/\sigma, \qquad a_1 = -(1 + a_0^2)/(2\sigma + 1), \tag{1.15a}$$

$$a_n(2\sigma + n) + \sum_{k=0}^{n-1} a_k a_{n-k-1} = 0, \qquad n = 2, 3, \ldots \,. \tag{1.15b}$$

Also

$$\alpha_0 = \sum_{n=0}^{\infty} \frac{a_n}{n+1} \rho^{n+1}. \tag{1.16}$$

The integration constant is zero in accordance with Eqs. (1.7).

The developments (1.14) and (1.16) can only be used for $\sigma = \sigma_1 = L + 1$. In the case of $\sigma = \sigma_2 = -L$, the coefficient of $a_{(2L)}$ in (1.15b) vanishes and the recurrence formula breaks down (for $\gamma = 0$, however, $a_{(2k)} = 0$, $k = 0, 1, \ldots$ and Eqs. (1.15) are still valid for $\sigma = \sigma_2$ (see Ref. [3])).

$d\alpha_{\sigma 2}/d\rho$ is determined in Section 3 by iteration.

2. Convergence of the Series for α_{σ_1} and $d\alpha_{\sigma_1}/d\rho$

Expand, by means of the binomial series, $d\alpha_{\sigma_1}^0/d\rho$ defined in (1.10). We find $d\alpha_{\sigma_1}^0/d\rho = \sum_{n=0} a_n^0 \rho^n$, where the $\{a_n^0\}$ can be obtained directly from Eq. (1.9) in the same way as the $\{a_n\}$ were derived from Eq. (1.3):

$$a_n^0 = a_n\,, \quad n = 1, 2; \quad a_n^0(2\sigma_1 + 1) + \sum_{k=0}^{n-1} a_k^0 a_{n-k-1}^0 = 0, \quad n = 2, 3, \ldots \,. \tag{2.1}$$

Now, as we shall prove below,

$$|\, a_k \,| \leqslant |\, a_k^0 \,|, \qquad k = 0, 1, \ldots \,. \tag{2.2}$$

Therefore,

$$\sum_{k=0}^{\infty} | a_k | \rho^k \leqslant \sum_{k=0}^{\infty} | a_k^0 | \rho^k. \tag{2.3}$$

But the expansion for $d\alpha_{\sigma_1}^0/d\rho$ (as the binomial series itself) converges absolutely and uniformly in any interval of the variable ρ where the inequalities

$$-1 < \frac{2\gamma}{\sigma_1} \cdot \frac{\rho}{\sigma_1 + \frac{1}{2}} - \left(\frac{\rho}{\sigma_1 + \frac{1}{2}}\right)^2 < +1 \tag{2.4}$$

are both satisfied. Conditions (2.4) are fulfilled for any ρ belonging to the interval $0 < \rho < \rho_1$ (see (1.11)) if $\sigma_1 > \gamma$.

Thus (see Ref. [4; p. 399]), by (2.3), the series (1.14) and (1.16) for $d\alpha_{\sigma_1}/d\rho$ and for α_{σ}. also converge uniformly and absolutely in $0 < \rho < \rho_1$ if

$$\sigma_1 > \gamma. \tag{2.5}$$

Consider now the proof of relations (2.2). From Eqs. (1.15) for $\sigma = \sigma_1$ and (2.1) it can be shown by induction that

$$a_k(\gamma) = -\left(-\frac{\gamma}{|\gamma|}\right)^{k+1} | a_k(\gamma)|, \quad a_k^0(\gamma) = -\left(-\frac{\gamma}{|\gamma|}\right)^{k+1} | a_k^0(\gamma)|, \quad k = 0, 1,\dots . \tag{2.6}$$

Suppose now that (2.2) are true for $k = 0, 1,\dots, n - 1$ with $n > 1$ and introduce (2.6) respectively into (1.15b) and (2.1). One has, since $2\sigma_1 + 1 < 2\sigma_1 + n$ for $n > 1$,

$$| a_n | = \frac{1}{2\sigma_1 + n} \sum_{k=0}^{n-1} | a_k | | a_{n-k-1} | \leqslant | a_n^0 |.$$

Relations (2.2), true for $k = 0, 1$ (see (2.1)), can now be established by mathematical induction.

TABLE I

L	γ	ρ	$d\alpha_{\sigma_1}/d\rho$	n	α_{σ_1}
10	0.5	1	$0.19755301 \times 10^{-2}$	7	$0.23706501 \times 10^{-1}$
10	5	1	0.40390207	9	0.42893424
30	5	10	$0.25552066 \times 10^{-2}$	15	0.81562269

Note. The truncated series $d\alpha_{\sigma_1}/d\rho = (1/\rho) \sum_{k=0}^{n-1} A_k$ and $\alpha_{\sigma_1} = \sum_{k=0}^{n-1} A_k/(k + 1)$ are used in the determination of $d\alpha_{\sigma_1}/d\rho$ and α_{σ_1}. The $A_k = a_k\rho^{k+1}$, $k = 0, 1,\dots, n - 1$ are obtained from A_0 and A_1 by recurrence (see (1.15b)) with $\sigma = L + 1$: $A_k[2(L + 1) + k] + \sum_{i=0}^{k-1} A_i A_{k-1-i} = 0$. The column headed by n gives the number of terms kept in the series for $d\alpha_{\sigma_1}/d\rho$ which satisfy the condition $\text{Max}(| A_{k-1} |, | A_k |) > \rho \times 10^{-8}$, so that $F_L(\gamma, \rho)$ can be calculated with 8 exact significant figures.

Table I shows $d\alpha_{\sigma_1}/d\rho$ and α_{σ_1} for different L, γ and ρ. In the examples given, $L \gg \rho$, $L \gg |\gamma|$ so that the conditions $0 < \rho < \rho_1$ and $\sigma_1 > \gamma$ are always satisfied.

The familiar, stable three-term recurrence formula (see Refs. [1], [2]) is used in the determination of $F_0(\gamma, \rho)$ from $F_L(\gamma, \rho)$ in Table II.

TABLE II

L	γ	ρ	$F_L(\gamma, \rho)$	$F_0(\gamma, \rho)$
10	0.5	1	$0.33554924 \times 10^{-10}$	0.51660150
10	5	1	$0.13750509 \times 10^{-13}$	$0.20413012 \times 10^{-4}$
30	5	10	$0.32745345 \times 10^{-14}$	0.91794492

Note. $F_L(\gamma, \rho)$ is obtained from (1.5). $F_{L-1}(\gamma, \rho)$ (necessary to the calculation of $F_0(\gamma, \rho)$ by recurrence) is obtained from $[1 + (\gamma/L)^2]^{1/2} F_{L-1} = [(2L + 1)/\rho + \gamma/L + d\alpha_{a_1}/d\rho] F_L$, derived from (1.5) and $[1 + (\gamma/L)^2]^{1/2} F_{L-1} = (L/\rho + \gamma/L + d/d\rho)F_L$ (see Ref. [1]).

3. Determination of $d\alpha_\sigma/d\rho$ by an Iterative Method

To simplify the notation, represent by $f', f'', ..., f^{(n)}$ the first n derivatives of any function f of ρ and write

$$b = \frac{d\alpha_\sigma}{d\rho}. \tag{3.1}$$

In accordance with these definitions, Eq. (1.3) becomes

$$\psi(b, b') = b^2 + b' + \frac{2\sigma}{\rho} b + 1 - \frac{2\gamma}{\rho} = 0. \tag{3.2}$$

The first approximation b_0 to b is taken equal to the function (1.10), i.e.,

$$b_0 = \frac{d\alpha_\sigma{}^0}{d\rho}. \tag{3.3}$$

Suppose now that b_n is a better approximation to b and write

$$h = b - b_n. \tag{3.4}$$

From (1.8), $h' \simeq h/\rho$, and $\psi(b, b') \simeq \psi(b_n + h, b'_n + h/\rho)$ or, expanding ψ by its Taylor's series up to terms of first order in h,

$$\psi(b, b') \simeq \psi(b_n, b'_n) + - \left[\left(\frac{\partial\psi}{\partial b}\right)_{(n)} + \frac{1}{\rho}\left(\frac{\partial\psi}{\partial b'}\right)_{(n)}\right], \tag{3.5}$$

where the subscript (n) means that the partial derivatives are taken at point (b_n, b'_n).

Since b is a solution of Eq. (3.2), $\psi(b, b') = 0$ in (3.5). The right-hand side of (3.5), however, is not necessarily zero, though we can make it vanish by substituting for b in (3.4) an appropriate new function b_{n+1} of ρ. We have, then,

$$b_{n+1} = b_n - \frac{\psi(b_n, b_n')}{\left(\frac{\partial\psi}{\partial b}\right)_{(n)} + \frac{1}{\rho}\left(\frac{\partial\psi}{\partial b'}\right)_{(n)}} \tag{3.6a}$$

or, by (3.2),

$$b_{n+1} = -\tfrac{1}{2}(b_n' - b_n{}^2 - b/\rho + 1 - 2\gamma/\rho)/[b_n + (\sigma + \tfrac{1}{2})/\rho], \qquad n = 0, 1, \ldots . \tag{3.6b}$$

Eq. (3.3) with Eqs. (3.6b) establish an iterative process for the determination of b $(= d\alpha_\sigma/d\rho)$.

Note that the calculation of b_n requires the first n derivatives of b_0, the first $n - 1$ derivatives of b_1,..., the first derivative of b_{n-1}. These functions are relatively simple to derive from Eqs. (3.3) and (3.6b) for n small. But it is better to find b_0' directly from Eq. (1.9):

$$b_0' = (b_0 - \gamma/\sigma)/[\rho + (\rho^2 b_0)/(\sigma + \tfrac{1}{2})]. \tag{3.7}$$

The $b_0^{(m)}$, $m = 2, 3, \ldots$ are obtained successively from (3.7).

Consider, now, the convergence of the iterative process. Subtract $\psi(b, b') = 0$ from $\psi(b_n, b_n')$ in the numerator of (3.6a) and develop $\psi(b, b') = \psi(b_n + h, b_n' + h')$ (see (3.4)) by its Taylor's series. We find

$$b - b_{n+1} = -\tfrac{1}{2}[(b - b_n)^2 + (b' - b_n') - (b - b_n)/\rho]/[b_n + (\sigma + \tfrac{1}{2})/\rho]. \tag{3.8}$$

Eq. (3.8) shows that the iterative process described above is a first order one. Thus, if b_a is an approximation to b, we have $b_a - b_n = M(b_n - b_{n-1})$, $b_a - b_{n-1} = M(b_{n-1} - b_{n-2})$ or, eliminating M,

$$b_a = \frac{b_n b_{n-2} - b_{n-1}^2}{b_n - 2b_{n-1} + b_{n-2}}. \tag{3.9}$$

Eq. (3.9) represents Aitken's δ^2-process and can be used to accelerate the convergence of the $\{b_n\}$ (see Ref. [2; p. 18]).

Table III illustrates the iterative process for $\sigma = \sigma_2 = -L$. The function b_a is obtained from (3.9) with $n = 3$.

TABLE III

L	γ	ρ	b_0	b_3	b_a
10	0.5	1	$0.26319435 \times 10^{-2}$	$0.26336925 \times 10^{-2}$	$0.26337165 \times 10^{-2}$
10	5	1	-0.43730346	-0.43744757	-0.43744757
30	5	10	$0.28262126 \times 10^{-2}$	$0.28319918 \times 10^{-2}$	$0.28320015 \times 10^{-2}$

Finally, we obtain $G_L(\gamma, \rho)$ from the Wronskian for this function and for $F_L(\gamma, \rho)$ (see Refs. [1, 2]) and from Eqs. (1.5). We find

$$F_L G_L \left(\frac{2L+1}{\rho} + \frac{d\alpha_{\sigma_1}}{d\rho} - \frac{d\alpha_{\sigma_2}}{d\rho}\right) = 1. \tag{3.10}$$

The examples shown in Table IV fulfill the conditions $0 < \rho < \rho_2$ (see (1.11) and $L + 1 > \gamma$ (see (2.5)). No attempt is made to obtain $G_0(\gamma, \rho)$ from $G_L(\gamma, \rho)$ by recurrence because such a "backward" process is numerically unstable.

TABLE IV

γ	ρ	L	$G_L(\gamma, \rho)$	L	$G_L(\gamma, \rho)$
0.5	1	10	$0.14191819 \times 10^{10}$	4	0.22443×10^{3}
5	1	10	$0.33296743 \times 10^{13}$	8	0.11777×10^{11}
5	10	30	$0.50065701 \times 10^{11}$	13	0.82766×10^{3}

Note. Both columns headed by $G_L(\gamma, \rho)$ are obtained from Eq. (3.10) taking $d\alpha_{\sigma_2}/d\rho \simeq b_a$, given by (3.9) with $n = 3$. The convergence of the iteration is not so good when L becomes closer to ρ and $|\gamma|$. That is why the 2nd column for $G_L(\gamma, \rho)$ shows only 5 exact significant figures.

All the calculations were performed in the Coimbra University Sigma 5 Xerox computer using a double-precision FORTRAN-IV programme.

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