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AN EXPANSION FOR COULOMB WAVE FUNCTIONS

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Abstract: An expansion for the regular radial Coulomb wave functions, as suggested by an iteration procedure on the wave equation, is developed and found to be more rapidly convergent than the customary expansions. Few terms suffice to give good accuracy for radial distances less than, or of the order of, the position of the classical turning point. This is true for all values of the orbital angular momentum no matter how high. No similar expansion has yet been developed for the irregular Coulomb wave functions.

1. Introduction

There is by now quite an impressive amount of literature (ref. [1a–d]) and others) dealing with Coulomb wave functions (hereafter called CWF-s). As is well known, these functions are expressible in terms of the confluent hypergeometric functions, and fairly extensive tabulations of them are now available [2]).

For some applications, however, for instance those which involve subsequent operations on CWF-s, it would still be very desirable to be able to obtain a simple and tractable form for these functions.

It is our aim in this paper to present briefly an expansion for the regular CWF-s, which is of a very simple nature and yet which converges much more rapidly than the usual expansions. For radial distances less than or about the position of the classical turning point only a few terms need be taken (however high the orbital angular momentum), thus yielding a simple representation of the CWF at least in this range.

The corresponding expansion for the irregular CWF-s has not, as yet, been obtained except in the simplest case of the irregular Bessel functions, i.e. for the zero value of the Coulomb parameter η.

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2. Regular CWF

The general radial CWF-s, denoted by $\bar{F}_L(\varrho; \eta)$, are defined [1a] as solutions of the radial Coulomb wave equation

$$\left[\mathscr{D}^2 + 1 - \frac{2\eta}{\varrho} - \frac{L(L+1)}{\varrho^2}\right]\bar{F}_L(\varrho; \eta) = 0, \tag{2.1}$$

where

$$\mathscr{D} \equiv d/d\varrho$$

and the symbols are the customary ones, viz.,

$$\varrho = kr = (2\pi \times \text{wave number}) \times (\text{radial distance}),$$

$\eta = ZZ'e^2/\hbar v$, v being the relative velocity of the two particles, and L is the orbital angular momentum quantum number.

In the present paper we shall confine our discussion almost exclusively to the study of regular solutions of (2.1) which we shall write in the usual way [1a, c] in the form

$$F_L(\varrho; \eta) = C_L(\eta)\varrho^{L+1}\,\Phi_L(\varrho; \eta) \tag{2.2}$$

where

$$C_L(\eta) = \frac{2^L}{(2L+1)!}\left\{(L^2+\eta^2)((L-1)^2+\eta^2)\ldots(1^2+\eta^2)\frac{2\pi\eta}{e^{2\pi\eta}-1}\right\}^{\frac{1}{2}} \tag{2.3}$$

and

$$\Phi_L(0; \eta) = 1. \tag{2.4}$$

On substituting (2.2) into (2.1), we immediately obtain

$$[\varrho\mathscr{D}^2 + 2(L+1)\mathscr{D} + \varrho - 2\eta]\Phi_L(\varrho; \eta) = 0. \tag{2.5}$$

It is evident from an examination of tabulations of regular CWF-s that the $\Phi_L(\varrho; \eta)$ are smooth and slowly varying functions of ϱ. For not too large values of ϱ, and particularly for high values of L, it should therefore be permissible to neglect, in a first approximation, the second order term $\varrho\,\mathscr{D}^2\Phi_L$ of (2.5) against the remaining terms.

On solving the resulting first order differential equation for $\Phi_L^{(1)}(\varrho; \eta)$, the first approximation to $\Phi_L(\varrho; \eta)$, we obtain

$$\Phi_L^{(1)}(\varrho; \eta) = \exp\left[\frac{\eta\varrho}{L+1} - \frac{\varrho^2}{4(L+1)}\right]. \tag{2.6}$$

In section 3 we shall discuss the accuracy of this function. In any event it can be improved quite efficiently if used as the starting step for an iteration procedure which we shall now describe.

We set up the successive approximation scheme as follows:

$$\varrho \mathscr{D}^2 \Phi_L^{(n-1)}(\varrho;\eta) + [2(L+1)\mathscr{D} + \varrho - 2\eta]\,\Phi_L^{(n)}(\varrho;\eta) = 0, \quad (2.7)$$

where $\Phi_L^{(n)}(\varrho;\eta)$ is the n^{th} approximation ($n = 1, 2, \ldots$) to $\Phi_L(\varrho;\eta)$, and $\Phi_L^{(0)}(\varrho;\eta)$ is chosen to be unity, by definition.

It is then clearly seen that, in general,

$$\Phi_L^{(n)}(\varrho;\eta) = W_L^{[4(n-1)]}(\varrho;\eta)\exp\left[\frac{\eta\varrho}{L+1} - \frac{\varrho^2}{4(L+1)}\right], \quad (2.8)$$

where the $W_L^{[m]}(\varrho;\eta)$ are m^{th} degree polynomials in ϱ; the first two W_L-s are

$$W_L^{(0)}(\varrho;\eta) = 1,$$

$$W_L^{(4)}(\varrho;\eta) = 1 + \frac{\varrho^2}{4(L+1)^2}\left(\frac{1}{2} - \frac{\eta^2}{L+1}\right) + \frac{\eta\varrho^3}{6(L+1)^3} - \frac{\varrho^4}{32(L+1)^3}.$$

The formula (2.8) suggests the possibility of an expansion

$$\Phi_L(\varrho;\eta) = \left(\sum_{\mu=0}^{\infty} a_{L,\mu}(\eta)\varrho^{\mu}\right)\exp\left[\frac{\eta\varrho}{L+1} - \frac{\varrho^2}{4(L+1)}\right] \quad (2.9)$$

for the exact solution of (2.5). It is apparent that (2.9) will be valid for all finite values of ϱ since both $\Phi_L(\varrho;\eta)$ and the $\exp[(\eta\varrho/(L+1)) - (\varrho^2/4(L+1))]$ have infinite radii of convergence and, furthermore, the exponential function has no zeroes for finite values of its argument. It thus follows that the series

$$\sum_{\mu=0}^{\infty} a_{L,\mu}(\eta)\varrho^{\mu} \quad (2.10)$$

must have an infinite radius of convergence.

Because of the initial requirement (2.4), we must have

$$a_{L,0}(\eta) \doteq 1. \quad (2.11)$$

On substituting (2.9) into (2.5), we therefore find for the first four $a_{L,\mu}$:

$$\left.\begin{aligned} a_{L,0} &= 1, \qquad & a_{L,2} &= \frac{L+1-2\eta^2}{4(L+1)^2(2L+3)}, \\ a_{L,1} &= 0, \qquad & a_{L,3} &= \frac{\eta[(L+1)^2+\eta^2]}{3(L+1)^3(L+2)(2L+3)}. \end{aligned}\right\} \quad (2.12)$$

In addition we obtain the general recurrence relationship

$$(\nu + 1)(\nu + 2(L + 1))a_{L,\nu+1} + \frac{1}{L+1}\left\{\eta\left[2\nu\, a_{L,\nu} - \frac{a_{L,\nu-2}}{L+1}\right] + \right.$$

$$\left. + \frac{2\eta^2 - (2\nu - 1)(L + 1)}{2(L + 1)} a_{L,\nu-1} + \frac{a_{L,\nu-3}}{4(L+1)}\right\} = 0, \quad (2.13)$$

for $\nu \geqq 3$, from which, e.g.,

$$a_{L,4} = -\frac{(4L + 1)(L + 1)^2(L + 2) + 4\eta^2[(7 - \eta^2)L + 10 - 2\eta^2]}{32(L + 1)^4\,(L + 2)(2L + 3)(2L + 5)}.$$

In the next section we investigate the convergence-rate of expansion (2.10) and compare it with the usual series expansion

$$\Phi_L(\varrho;\eta) = \sum_{\varkappa=0}^{\infty} A_{L,\varkappa}(\eta)\varrho^{\varkappa}. \quad (2.14)$$

Here the coefficients $A_{L,\varkappa}$ satisfy the recurrence relation

$$A_{L,\varkappa} = \frac{2\eta A_{L,\varkappa-1} - A_{L,\varkappa-2}}{\varkappa(2L + \varkappa + 1)}, \quad (2.15)$$

so that

$$\left.\begin{aligned} A_{L,0} &= 1, & A_{L,2} &= \left\{\frac{2\eta^2}{L+1} - 1\right\}\frac{1}{2(2L+3)}, \\ A_{L,1} &= 0, & A_{L,4} &= \frac{\eta[2\eta^2 - 3L - 4]}{6(L+1)(L+2)(2L+3)}, \text{ etc.} \end{aligned}\right\} \quad (2.16)$$

We shall see in section 3 that the series (2.10) is much more rapidly convergent than (2.14).

We shall close this section with a mention of the irregular solutions of (2.1), i.e. the functions

$$G_L(\varrho;\eta) = D_L(\eta)\varrho^{-L}\Theta_L(\varrho;\eta) \quad (2.17)$$

with

$$D_L = \frac{1}{(2L + 1)C_L},$$

and where the function Θ_L may be expressed in the form

$$\Theta_L(\varrho;\eta) = \Psi_L(\varrho;\eta) + \varrho^{2L-1}(p_L(\eta)\ln 2\varrho + q_L(\eta))\Phi_L(\varrho;\eta). \quad (2.18)$$

Here Ψ_L is a well-behaved function of ϱ such that

$$\Psi_L(0;\eta) = 1, \quad (2.19)$$

and $p_L(\eta)$, $q_L(\eta)$ are functions of L, η such that

$$p_L(0) = q_L(0) = 0. \quad (2.20)$$

It is evident that we cannot apply to $\Theta_L(\varrho;\eta)$ itself (for a general η) any procedure analogous to the one we have employed successfully in the case of $\Phi_L(\varrho;\eta)$. This is so since the additive term containing a logarithmic factor $\ln 2\varrho$ *cannot* be represented by a power series in ϱ. We may, however, still use a corresponding treatment for the function $\Psi_L(\varrho;\eta)$ alone. We hope to be able to deal fully with this problem in a later publication.

We note, however, from (2.18) with (2.20) that in the case of $\eta = 0$

$$\Theta_L(\varrho; 0) = \Psi_L(\varrho; 0)$$

is a *regular* function and satisfies the equation

$$(\varrho\mathscr{D}^2 - 2L\,\mathscr{D} + \varrho)\,\Theta_L(\varrho; 0) = 0. \tag{2.21}$$

Comparing (2.21) with (2.5) and then (2.17) with (2.2), and remembering that both F_L and G_L are solutions of (2.1), we may conclude that, at least formally, we can obtain $\Theta_L(\varrho; 0)$ from $\Phi_L(\varrho; 0)$ on replacing everywhere $(L+1)$ by $(-L)$. An exact calculation similar to the one made in the case of Φ_L does, in fact, lead us to the same result. It gives

$$\Theta_L(\varrho; 0) = \left(\sum_{\mu=0}^{\infty} b_{L,\mu}\varrho^{\mu}\right) \exp\left(\frac{\varrho^2}{4L}\right), \tag{2.22}$$

for $L \neq 0$, where

$$\begin{aligned} b_{L,0} &= 1, & b_{L,2} &= \frac{1}{4L(2L-1)}, \\ b_{L,1} &= 0, & b_{L,3} &= 0, \end{aligned} \tag{2.23}$$

with the general recurrence relation

$$(\nu+2)(\nu-2L+1)b_{L,\nu+2} + \frac{1}{2L}\left\{(2\nu+1)b_{L,\nu} + \frac{b_{L,\nu-2}}{2L}\right\} = 0 \tag{2.24}$$

for $\nu = 2, 4, \ldots$, all the b's for odd ν vanishing identically.

The convergence of the series

$$\sum_{\mu=0}^{\infty} b_{L,\mu}\varrho^{\mu}$$

will be essentially identical to the corresponding $\eta = 0$ case of (2.10) which is considered in section 3; in analogy with (2.10) therefore we know that the above series is quite rapidly convergent for distances of order of or less than the classical turning point. Of course, eq. (2.22) and, when $\eta = 0$, also eq. (2.9) are essentially representations of the well known spherical Bessel functions which are not only amply tabulated, but are made up of elementary trigonometrical functions. Even in this case, however, eq. (2.9) and (2.22) may find application, for example in coding problems for an electronic computer. For high L values it may be very convenient to use a rapidly convergent series in which no great cancellation occurs, rather than to code the machine to calculate spherical Bessel functions from their exact expressions, which for distances inside the classical turning point involve cancellations to a very high degree.

3. Rate of Convergence of Series

The fact that the series (2.9) is, in general, quite rapidly convergent at least for distances less than or of order of the classical

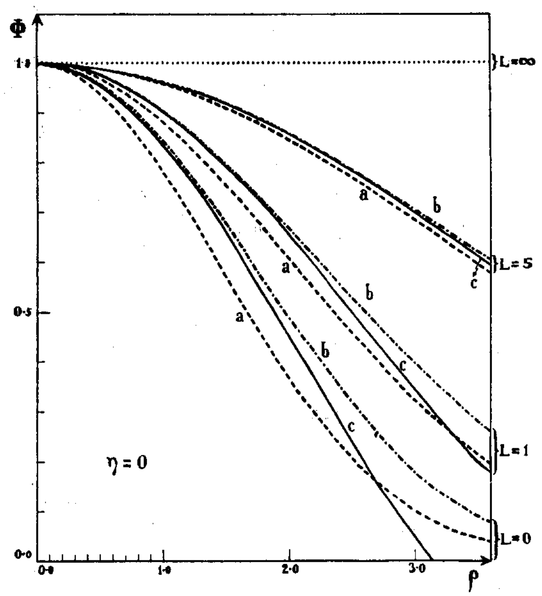

Fig. 1. Curves representing the approximations $\Phi_L^{(1)}(\varrho; 0)$ and $(1 + a_{L,2}(0)\varrho^2)\Phi_L^{(1)}(\varrho; 0)$ and marked respectively as **a** and **b**, are plotted together with the exact function $\Phi_L(\varrho; 0)$ — curve **c** — for values of $L = 0$, 1, and 5. The line $\Phi_\infty^{(1)}(\varrho; 0) \equiv \Phi_\infty(\varrho; 0) = 1$ has been *dotted* in for comparison. Note the fast improvement of the approximations with increasing L.

turning point is illustrated by the curves of Figs. 1, 2, and 3. In Figs. 1 and 2 we have plotted the results yielded by (2.9) when only the first term of the series is taken, and also when a few additional terms are included. The resulting curves are compared with those corresponding to the exact function Φ_L. Fig. 1 corresponds to the case $\eta = 0$, and Fig. 2 to the case $\eta = 2$, and in each case we have considered the three values 0, 1, and 5 for L.

In Fig. 3 the exact function Φ_L is compared to the simple function $\Phi_L^{(1)}$ yielded by the first term of (2.9) for the cases $L = 5, \eta = 0, 1, 2$.

From the illustrative examples of Figs. 1 and 2 we see that for values of ϱ corresponding to distances less than the classical turning point, a quite rapid convergence is achieved. The reason for this, of

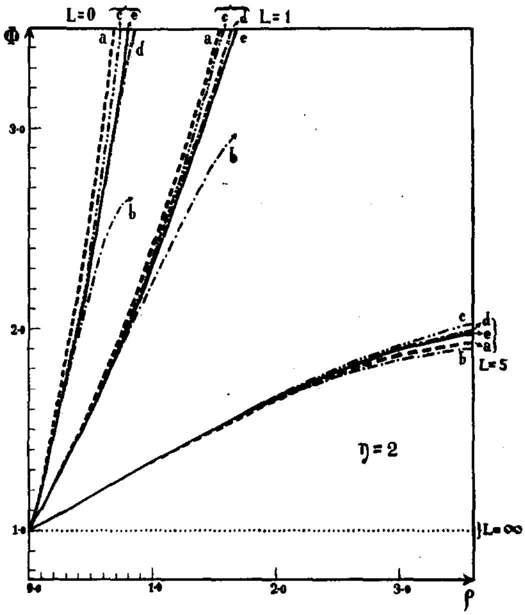

Fig. 2. Curves representing the approximations $\Phi_L^{(1)}$ $(\varrho; 2)$ and $(1+\sum_{\nu=2}^{r+2} a_{L,\nu}(2)\varrho^\nu)\Phi_L^{(1)}$ $(\varrho; 2)$ with $r = 0$, 1, and 2 and marked consecutively **a** to **d**, are plotted together with the exact function $\Phi_L(\varrho; 2)$ — curve **e** — for values of $L = 0$, 1, and 5. The line $\Phi_\infty^{(1)}$ $(\varrho; 2) \equiv \Phi_\infty(\varrho; 2) = 1$ has been *dotted* in for comparison. An arrow at the end-point of a curve (when within the frame of the graph) indicates that this curve is discontinued since it starts to deviate violently at this point from the corresponding exact function.

course, is that the multiplying factor $\Phi_L^{(1)}$ of (2.9) is itself a quite reasonable first approximation (see also Fig. 3) so that the series of (2.9) plays the role merely of a correction factor, at least for the distances discussed.

The reasons why the multiplying factor $\Phi_L^{(1)}$ is a good first approximation may be readily seen. We note that, apart from the trivial relation

$$\Phi_L^{(1)}(0;\eta) = \Phi_L(0;\eta),$$

we also have (actually as an immediate consequence of our method of deriving (2.6)),

$$\left[\frac{\partial}{\partial\varrho}\Phi_L^{(1)}(\varrho;\eta)\right]_{\varrho=0} = \left[\frac{\partial}{\partial\varrho}\Phi_L(\varrho;\eta)\right]_{\varrho=0}.$$

Also, $\Phi_L^{(1)}(\varrho;\eta)$ is a Gaussian in ϱ with its maximum

$$\lambda(L,\eta) = \exp\left(\frac{\eta^2}{L+1}\right)$$

situated at

$$\bar{\varrho}(\eta) = 2\eta$$

and with a width parameter

$$\sigma(L) = (2(L+1))^{\frac{1}{2}}.$$

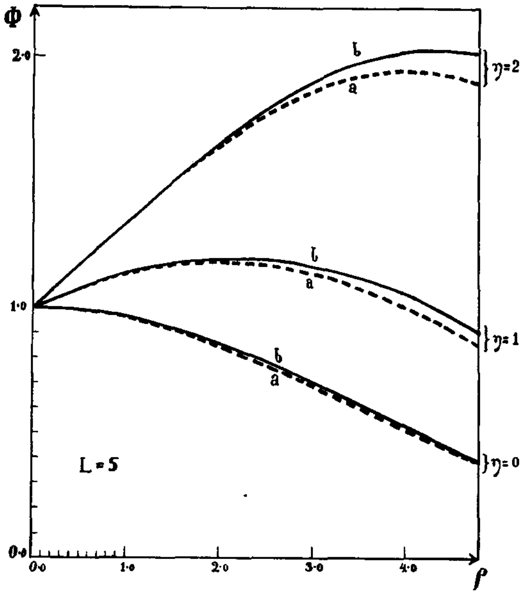

Fig. 3. Curves representing $\Phi_5^{(1)}(\varrho;\eta)$ and $\Phi_5(\varrho;\eta)$ and marked respectively as **a** and **b**, are plotted for values of $\eta = 0$, 1, and 2. Note how the position and height of peaks vary with η.

All the qualitative consequences of these features are true for the half-width, position, and variation with L and η of the first maximum of the exact function $\Phi_L(\varrho;\eta)$.

As may easily be verified, a very large number of terms of the usual series (2.14) must be summed to give accuracy comparable with the first one or two terms of our expression (2.9), particularly for large values of L.

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