Numerical Treatment of Coulomb Wave Functions

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A number of methods, suitable for computation of Coulomb wave functions with high accuracy, are collected, most of them previously well known. It is shown that the regions where these methods can be used, together cover all positive values of ρ and η in the case $L=0$. All formulas are presented in a form well adapted for direct numerical computation.

1. INTRODUCTION

As is well known, Coulomb wave functions appear in many problems of great physical interest, especially in scattering problems involving charged particles. It is quite natural that many articles have been published on this subject. In the beginning the interest centered around obtaining different representations of the functions, and in this connection we only mention works by Sexl[1] and by Yost, Wheeler, and Breit.[2] (An extensive bibliography can be found in the NBS table.[3]) During the last years one has become more and more interested in questions concerning numerical problems related to these functions. This is not surprising since a physicist working in this field is likely to desire an answer to the question: With a given set of values of ρ, η, and L, how can the numerical values of the functions and their derivatives be obtained? Do tables exist for this region, and, if not, which method should be used in order to obtain reasonably accurate values with a reasonable amount of work? It is the aim of the present paper to give an answer to these questions, and the given formulas will in general admit at least 5–6 digits accuracy.

2. NOTATIONS

The differential equation, written in standard form, is

$$d^2y/d\rho^2+(1-2\eta/\rho-L(L+1)/\rho^2)y=0. \qquad (2.1)$$

We suppose throughout the paper that ρ and η are positive and L a positive integer. The solutions are chosen in the following way: $F_L(\eta,\rho)=0$ for $\rho=0$; the amplitude of $F_L\to 1$ when $\rho\to\infty$. It can be shown that

$$F_L\sim\sin\left[\rho-\eta\log 2\rho-\frac{L}{2}\pi+\sigma_L\right]=\sin\theta_L,$$

where $\sigma_L=\arg\Gamma(i\eta+L+1)$, when $\rho\to\infty$. Then the other solution $G_L(\eta,\rho)$ is defined by its asymptotic behavior: $G_L(\eta,\rho)\sim\cos\theta_L$, when $\rho\to\infty$. A useful integral representation is the following:

$$F_L+iG_L=ie^{-i\rho}[(2L+1)!C_L\rho^L]^{-1}\cdot\int_0^\infty t^{L-i\eta}(t+2i\rho)^{L+i\eta}\cdot e^{-t}dt \qquad (2.2)$$

with

$$C_L\equiv(2^L/(2L+1)!)\cdot\{(1+\eta^2)\cdots(L^2+\eta^2)\}^{\frac{1}{2}}\cdot\{2\pi\eta/(e^{2\pi\eta}-1)\}^{\frac{1}{2}}. \qquad (2.3)$$

Further D_L is defined through $C_LD_L=1/(2L+1)$.

In what follows, F' and G' stand for $dF/d\rho$ and $dG/d\rho$, respectively. Further ϕ_L and Θ_L are defined through $F_L=C_L\rho^{L+1}\cdot\phi_L$; $G_L=D_L\rho^{-L}\Theta_L$.

3. RECURRENCE RELATIONS

The Coulomb wave functions depend on three variables ρ, η, and L. However, by making use of the assumption that L is an integer, it turns out that, e.g., F_{L+1} can be computed if F_L and F_L' are known, and consequently, it suffices in principle to compute F_0, F_0', G_0, and G_0'. Recurrence formulas, obtained from the integral representation, were given by Powell.[4] It was pointed out by Infeld,[5] however, that the recurrence relations only depend upon the differential equation and can be obtained as special cases of a factorization method.[6]

The following elementary proof may also be of some interest. We try the representation

$$u_{L-1}=(a+b/\rho)u_L+cu_L'$$

where u_L and u_{L-1} are any solutions of the corresponding differential equations. Then making use of the differential equations for u_L and u_{L-1} the following condition is easily obtained:

$$\{aL-c\eta+(b-cL)(L+1)/\rho\}u_L-(b-cL)u_L'\equiv 0$$

from which we conclude

$$u_{L-1}=\text{const}\{(\eta/L+L/\rho)u_L+u_L'\}.$$

[1] T. Sexl, Z. Physik **56**, 72 (1929).
[2] Yost, Wheeler, and Breit, Phys. Rev. **49**, 174 (1936).
[3] *Tables of Coulomb Wave Functions*, Vol. I. NBS, Appl. Math. Series **17** (Washington, D. C., 1952).
[4] John L. Powell, Phys. Rev. **72**, 626 (1947).
[5] L. Infeld, Phys. Rev. **72**, 1125 (1947).
[6] L. Infeld and T. E. Hull, Revs. Modern Phys. **23**, 21 (1951).

The constant is the only thing which depends explicitly on the definition of the solution. The following relations are the most important ones (u_L now stands for F_L or G_L):

$$(\eta^2+L^2)^{\frac{1}{2}}u_{L-1}/L=(\eta/L+L/\rho)u_L+u_L' \quad (3.1)$$

$$(\eta^2+(L+1)^2)^{\frac{1}{2}}u_{L+1}/(L+1) = (\eta/(L+1)+(L+1)/\rho)u_L-u_L' \quad (3.2)$$

$$(\eta^2+(L+1)^2)^{\frac{1}{2}}u_{L+1}/(L+1)+(\eta^2+L^2)^{\frac{1}{2}}u_{L-1}/L = (2L+1)(\eta/L(L+1)+1/\rho)u_L. \quad (3.3)$$

To these formulas we may add the Wronskian relation

$$F_L'G_L-F_LG_L'\equiv 1. \quad (3.4)$$

Substituting F_L', G_L' expressed in F_{L-1}, F_L and G_{L-1}, G_L, respectively, from (3.1) we obtain

$$F_{L-1}G_L-G_{L-1}F_L\equiv L/(\eta^2+L^2)^{\frac{1}{2}}. \quad (3.5)$$

Both relations are useful for checking purposes.

From (3.1) and (3.2) we can form a pair of equations in $v_1=u_L+u_{L-1}$; $v_2=u_L-u_{L-1}$;

$$\{L/\rho-((\eta^2+L^2)^{\frac{1}{2}}-\eta)/L\}v_1+v_2'=0$$

$$\{L/\rho+((\eta^2+L^2)^{\frac{1}{2}}+\eta)/L\}v_2+v_1'=0$$

which integrated numerically will give u_L, u_{L-1}, u_L', and u_{L-1}' at the same time.

As is shown in reference 3 the recurrence relations can be used over a large range of values of L without too serious accumulation of error. A practical scheme is presented in a recent paper by T. Stegun and M. Abramowitz.[7]

In what follows we restrict ourselves to the case $L=0$ unless otherwise is mentioned.

4. TABLES

The most extensive table so far is the NBS table,[3] prepared under the direction of M. Abramowitz. This table deals with the function F_L for $L=0(1)5$, 10, 11, 20, and 21; $\eta=-5(1)5$ and $\rho=0(0.2)5$ with complete interpolation facilities in η. Most of the entries are given with an accuracy of seven digits or more. Further the volume contains three extremely useful auxiliary tables: R.P. $(\Gamma'(1+i\eta)/\Gamma(1+i\eta))$; $\sigma_0=\arg\Gamma(1+i\eta)$; C_0 [defined in (2.3)].

Recently a small table containing F_0, F_0', G_0, and G_0' for $\rho=2\eta$ has also been published.[8]

These tables have partly superseded a previous one[9,10] which deals with the regular as well as the irregular function for $L=0(1)4$, $0<\eta<4$, and $0<\rho<6$. The accuracy lies between 0.1 and 2.2%. A small table of G_0 and G_0' for $0<\rho,\eta\leq 1$ is given in a previous work.[11]

Recently a "skeleton table"[12] of f_L, g_L, f_L', and g_L' [defined in (5.2) and (5.5)] has been published for $L=0$ and $L=5$ and for $\rho,\eta=0(1)10$. The table also contains the five first reduced η-derivatives. Unfortunately this table has some drawbacks, mostly due to the method of computation [numerical quadrature, formulas (5.2) and (5.5)]. First: for high values of η and small values of ρ the accuracy of the regular function and its derivative is unacceptable. Second: in many cases interpolation in η with $\Delta\eta$ close to $\frac{1}{2}$ is not sufficiently accurate. (Numerical example: $L=5$, $\rho=9$, $\eta=5.5$: $g_5=32.23474$ as obtained from $\eta=5$ and $g_5=32.16459$ as obtained from $\eta=6$, the correct value probably being about 32.249.) Third: the functional values as a rule are given with lower accuracy for $L=0$ than for $L=5$.

The irregular function does not present any special difficulties in this respect. Throughout the region it is given with an accuracy of 5–6 digits for $L=0$ and of 7–8 digits for $L=5$. If necessary at least one extra digit can be obtained for $L=0$ by taking the corresponding values for $L=5$ and using the recurrence relations. The regular function on the other hand presents a more complicated picture, and the scheme of Fig. 1 is recommended.

5. INTEGRAL REPRESENTATION

From (2.2) and (2.3) we easily find the following formulas:

$$F_L=A_L\rho^{L+1}f_L;\quad G_L=A_L\rho^{L+1}g_L \quad (5.1)$$

with

$$\begin{cases} f_L=\int_0^\infty (1-th^2\xi)^{L+1}\cos(\rho th\xi-2\eta\xi)d\xi & (5.2a) \\ g_L=\int_0^\infty (1+\xi^2)^L e^{-\rho\xi+2\eta\,\mathrm{arctg}\xi}d\xi \\ \qquad -\int_0^\infty (1-th^2\xi)^{L+1}\cdot\sin(\rho th\xi-2\eta\xi)d\xi & (5.2b) \end{cases}$$

and

$$A_L=2^{-L}(1-e^{-2\pi\eta})^{\frac{1}{2}} \cdot\{2\pi\eta\cdot(1^2+\eta^2)(2^2+\eta^2)\cdots(L^2+\eta^2)\}^{-\frac{1}{2}}. \quad (5.3)$$

In particular we have for $L=0$:

$$A_0=\{(1-e^{-2\pi\eta})/2\pi\eta\}^{\frac{1}{2}}. \quad (5.4)$$

Formula (5.2a) can also only be used in the transition region, while (5.2b) can be used in the whole region between the transition line and the line $\rho=0$. The derivatives

[7] T. Stegun and M. Abramowitz, Phys. Rev. **98**, 1851 (1955).
[8] M. Abramowitz and P. Rabinowitz, Phys. Rev. **96**, 77 (1954).
[9] Bloch, Hull, Broyles, Bouricius, Freeman, and Breit, Phys. Rev. **80**, 553 (1950).
[10] Bloch, Hull, Broyles, Bouricius, Freeman, and Breit, Revs. Mod. Phys. **23**, 147 (1951).
[11] C. E. Fröberg, Arkiv Fysik **3**, 13 (1951).
[12] C. E. Fröberg and P. Rabinowitz, *Tables of Coulomb Wave Functions;* NBS, Report 3033 (1954).

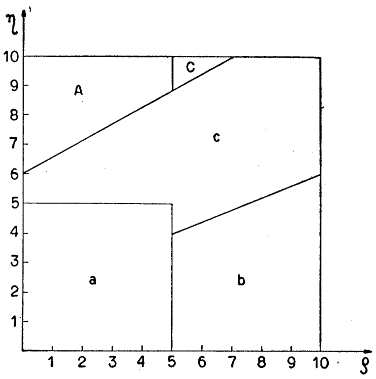

FIG. 1. Regions where different methods for obtaining the regular function are recommended. *a*: Use the table in reference 3. *b*: Use the table for $L=0$ in reference 12 or if higher accuracy is needed the same method as in *c*. *c*: Use the table for $L=5$ in reference 12 and the recurrence relations. *A*: Use 7, 10, 12. *C*: Use 9. 1, 2, 3.

can be computed directly:

$$\begin{cases} f_L' = -\displaystyle\int_0^\infty th\xi\cdot(1-th^2\xi)^{L+1}\sin(\rho th\xi - 2\eta\xi)d\xi & (5.5a) \\ g_L' = -\displaystyle\int_0^\infty \xi(1+\xi^2)^L e^{-\rho\xi+2\eta\,\mathrm{arctg}\,\xi}d\xi & \\ \qquad -\displaystyle\int_0^\infty th\xi(1-th^2\xi)^{L+1}\cdot\cos(\rho th\xi-2\eta\xi)d\xi. & (5.5b) \end{cases}$$

Note that, e.g., $F_L' = A_L\rho^{L+1}\{f_L' + (L+1)f_L/\rho\}$.

The great advantage of these expressions is that the successive reduced derivatives with respect to η can be obtained without difficulty. More extensive computations, however, are prohibitive unless a fast electronic computing machine is used. It turns out that (5.2) and (5.5) in general only need to be used in region D (Fig. 2), and even here one has a choice between these quadrature formulas and numerical integration of Eq. (2.1).

6. NUMERICAL INTEGRATION

If a large number of functional values with the same η but different values of ρ are needed, it might be convenient first to compute a key value and then integrate numerically (using the higher derivatives which are easily obtained). Otherwise this method should be used only for the region D in competition with the quadrature, mentioned in Sec. 5, and possibly very close to the transition line $\rho=2\eta$.

In this connection it should be observed that both F and G vary extremely rapidly to the left of the transition line, and this fact strongly affects the errors due to truncation and round-off. For example, when integrating F in the direction of decreasing values of ρ, a small error means an admixture of G, and since G is rapidly increasing, the effect will be that F will soon disappear compared with the error.

If it is necessary to integrate numerically over wide ranges in this region, the following transformations are

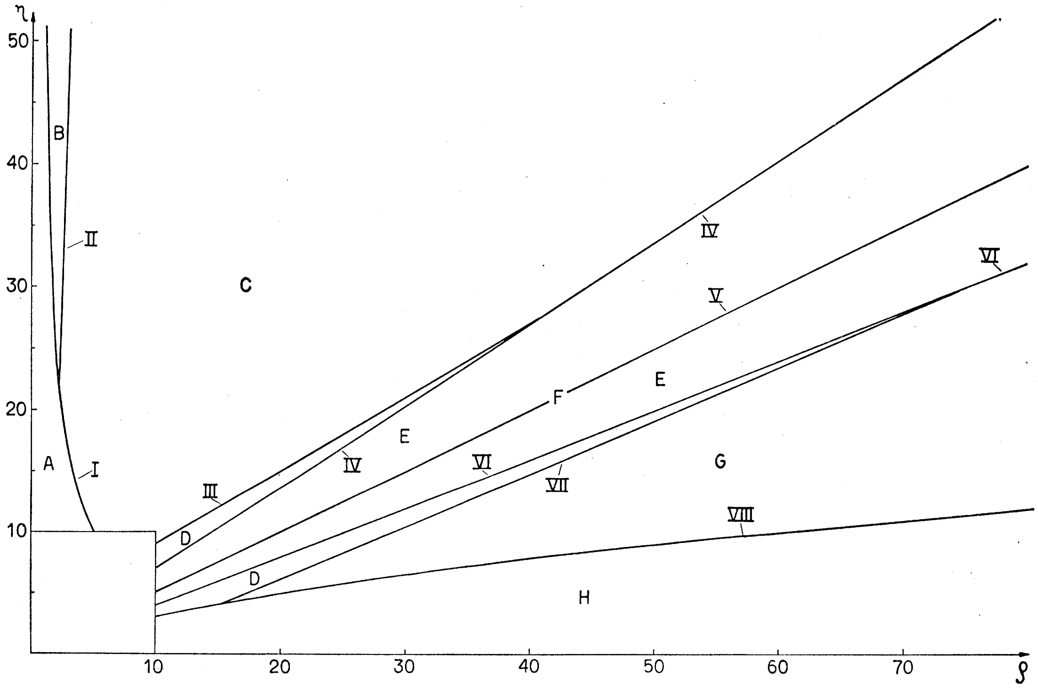

FIG. 2. Regions where different methods of computation should be used. For closer explanation, consult Table I at the end of the paper.

suggested:

$$\begin{cases} \psi_1=\log F_L-(L+1)\log\rho-\log C_L \\ \psi_2=\rho F_L'/F_L-(L+1) \\ \psi_3=\log G_L+L\log\rho-\log D_L \\ \psi_4=\rho G_L'/G_L+L. \end{cases} \tag{6.1}$$

Then we obtain the equations:

$$\begin{cases} \psi_1'=\psi_2/\rho \\ \psi_2'=2\eta-\rho-\psi_2^2/\rho-(2L+1)\psi_2/\rho \\ \psi_3'=\psi_4/\rho \\ \psi_4'=2\eta-\rho-\psi_4^2/\rho+(2L+1)\psi_4/\rho \end{cases} \tag{6.2}$$

with the initial values $\psi_1(0)=\psi_2(0)=\psi_3(0)=\psi_4(0)=0$ and the Wronskian relation

$$(\psi_2-\psi_4+2L+1)\cdot e^{\psi_1+\psi_3}\equiv 2L+1. \tag{6.3}$$

The functions ψ vary much more slowly and smoothly than do the functions F and G. As an example we give the following values for $\eta=100$ and $L=0$:

$$\psi_1(0)=0;\quad \psi_1(1)=23.0092;\quad \psi_1(4)=50.0988.$$

7. THE POWER SERIES EXPANSIONS

The essential formulas for the power series expansions were given by Yost, Wheeler, and Breit[2] and are collected in a compact form in reference 3. Here we will present them arranged in a way which is convenient for numerical work.

First we introduce some notations.

$$p_0=2\eta;\quad p_L=\frac{2\eta(1+\eta^2)(4+\eta^2)\cdots(L^2+\eta^2)\cdot 2^{2L}}{(2L+1)\cdot[(2L)!]^2} \tag{7.1}$$

$$\omega_L=\log 2\rho+q_L/p_L \tag{7.2}$$

where the general expression of q_L/p_L can be found in reference 3, p. XVI. The first six values are given below.

$$\begin{cases} q_0/p_0=f(\eta)+2C-1 \\ q_1/p_1=f(\eta)+2C-11/6+1/4(1+\eta^2) \\ q_2/p_2=f(\eta)+2C-137/60 \\ \qquad +(4\eta^2+13)/8(1+\eta^2)(4+\eta^2) \\ q_3/p_3=f(\eta)+2C-\dfrac{363}{140}+\dfrac{6\eta^4+69\eta^2+150}{8(1+\eta^2)(4+\eta^2)(9+\eta^2)} \\ q_4/p_4=f(\eta)+2C-\dfrac{7129}{2520} \\ \qquad +\dfrac{16\eta^6+428\eta^4+3124\eta^2+5637}{16(1+\eta^2)(4+\eta^2)(9+\eta^2)(16+\eta^2)} \\ q_5/p_5=f(\eta)+2C-\dfrac{83711}{27720} \\ \qquad +\dfrac{20\eta^8+1020\eta^6+16680\eta^4+98105\eta^2+158295}{16(1+\eta^2)(4+\eta^2)(9+\eta^2)(16+\eta^2)(25+\eta^2)}. \end{cases} \tag{7.3}$$

Here $f(\eta)=\text{R.P.}\ (\Gamma'(1+i\eta)/\Gamma(1+i\eta))$ (tabulated in reference 3) and $C=$ Euler's constant $=0.5772156649\cdots$.

The expansions then run as follows:

$$\begin{cases} (n+1)(n+2L+2)B_{n+1}=2\eta\rho B_n-\rho^2 B_{n-1} & (7.4) \\ (n+1)(n-2L)P_{n+1}=2\eta\rho P_n-\rho^2 P_{n-1} \\ \qquad -(2n-2L+1)p_L\rho^{2L+1}B_{n-2L} & (7.5) \end{cases}$$

$$\text{with} \begin{cases} B_0=1 \\ B_1=\eta\rho/(L+1) \end{cases} \text{and} \begin{cases} P_0=1 \\ P_{2L+1}=0. \end{cases}$$

We now define six quantities, B, S, P, R, Q, and T:

$$\begin{cases} B=\sum B_k\ (=\phi_L) \quad S=\sum kB_k \\ P=\sum P_k \quad R=\sum kP_k \\ Q=p_L\omega_L\rho^{2L+1}B+P\ (=\Theta_L) \\ T=p_L\rho^{2L+1}\{[1+(2L+1)\omega_L]B+\omega_L\cdot S\}+R \end{cases} \tag{7.6}$$

and from these values we can obtain the functional values directly:

$$\begin{cases} F_L=C_L\rho^{L+1}\cdot B \\ F_L'=C_L\rho^L[(L+1)B+S] \\ G_L=D_L\rho^{-L}\cdot Q \\ G_L'=D_L\rho^{-L-1}[-LQ+T]. \end{cases} \tag{7.7}$$

It is also interesting to note that the functions ψ_1, ψ_2, ψ_3, ψ_4 introduced in Sec. 6 can be written in a very simple form:

$$\begin{cases} \psi_1=\log B \\ \psi_2=S/B \\ \psi_3=\log Q \\ \psi_4=T/Q. \end{cases} \tag{7.8}$$

The Wronskian relation has the form

$$BQ+(SQ-BT)/(2L+1)\equiv 1. \tag{7.9}$$

In particular we have for $L=0$,

$$\begin{cases} (n+1)(n+2)B_{n+1}=2\eta\rho B_n-\rho^2 B_{n-1} & (7.10) \\ n(n+1)P_{n+1}=2\eta\rho P_n-\rho^2 P_{n-1}-(2n+1)2\eta\rho B_n & (7.11) \end{cases}$$

with $B_0=1$, $B_1=\eta\rho$; $P_0=1$; $P_1=0$. Further:

$$Q=2\eta\rho(\log 2\rho+2C-1+f(\eta))B+P$$

$$T=2\eta\rho\{B+(\log 2\rho+2C-1+f(\eta))(B+S)\}+R$$

$$\begin{cases} F_0=C_0\rho\cdot B;\quad F_0'=C_0(B+S) \\ G_0=Q/C_0;\quad G_0'=T/C_0\rho. \end{cases} \tag{7.12}$$

It is easy to see that the power series expansions should not be used if $\eta\rho$ or ρ^2 are very large. A reasonable choice seems to be

$$\eta\rho \leq 50; \quad \rho \leq 10 \tag{7.13}$$

which corresponds to region A in Fig. 2. If $\rho=5$, $\eta=10$ about 20 terms are necessary to obtain 7 digits accuracy. However, because of the very simple formation law of the successive terms, in some cases it may be reasonable to go beyond these limits.

8. THE BESSEL-CLIFFORD EXPANSION

Expansions of both regular and irregular Coulomb wave functions in terms of Bessel-Clifford functions (i.e., essentially modified Bessel functions) are important for large values of η and small values of ρ. Such expansions have been obtained by Breit and Hull[13,14] and by Abramowitz.[15–17] We shall here give these expansions in a form more convenient for numerical calculations.

In reference 16 Abramowitz derived an expansion for $\phi_L(\eta,\rho)$. We shall first give the corresponding expression for the irregular function. In Eq. (2.1) we make the transformations: $x^2=8\eta\rho$; $y=G_L=x\cdot\Gamma_L$, from which we get

$$\frac{d^2\Gamma_L}{dx^2}+\frac{1}{x}\frac{d\Gamma_L}{dx}-\left(1+\frac{(2L+1)^2}{x^2}-\frac{x^2}{16\eta^2}\right)\Gamma_L=0. \tag{8.1}$$

If the term $x^2/16\eta^2$ is discarded, we obtain an equation with the general solution: $c_1I_{2L+1}(x)+c_2K_{2L+1}(x)$. Now it has been proved by Yost, Wheeler, and Breit that for small values of x

$$G_L \sim \frac{(2\eta)^L}{(2L)!}D_L\cdot x\cdot K_{2L+1}(x) \tag{8.2}$$

and this leads us to try the following expansion:

$$\Gamma_L=K_{2L+1}+\sum_{s=1}^{\infty}a_s x^{s+1}\cdot K_{2L-s}. \tag{8.3}$$

Then we find:

$$a_1=L/16\eta^2;\quad a_2=1/96\eta^2;\quad a_3=L(L-1)/512\eta^4;$$
$$32\eta^2(s+4)a_{s+3}=2(2L-s-2)a_{s+1}+a_s;\qquad s=1,2,3,\cdots. \tag{8.4}$$

A remaining multiplicative constant is easily found to be unity. Thus we have

$$G_L=\frac{(2\eta)^L}{(2L)!}\cdot D_L\cdot x\cdot \Gamma_L. \tag{8.5}$$

In reference 17 Abramowitz has obtained expansions for ϕ_L in terms of $I_n(x)$ and for Θ_L in terms of $K_n(x)$ ($n=2L+1, 2L+2, \cdots$) with the same coefficients except for a factor $(-1)^n$. It is interesting to note that in these formulas Θ_L must be provided with a numerical factor ($\neq 1$), while in the other set of formulas (reference 16, Eq. (3.15)) and formula (8.5) which has just been proved, such a factor must be appended to ϕ_L.

From now on we restrict ourselves to the case $L=0$. First we introduce some new notations:

$$\begin{cases} F_0=C_0(4\eta)^{-1}\cdot x\cdot\Lambda_0 \\ F_0'=C_0M_0 \\ G_0=D_0\cdot x\Gamma_0 \\ G_0'=D_0\cdot 4\eta\cdot N_0. \end{cases} \tag{8.6}$$

As is easily found we have

$$M_0=\left(\frac{d}{dx}+\frac{1}{x}\right)\Lambda_0 \quad\text{and}\quad N_0=\left(\frac{d}{dx}+\frac{1}{x}\right)\Gamma_0.$$

Putting $\epsilon=(16\eta^2)^{-1}$ we can write the expansions in the following form:

$$\begin{aligned}\Lambda_0=I_1&+\epsilon\left[-\frac{x^3}{6}I_2\right]+\epsilon^2\left[\frac{x^5}{10}I_4+\frac{x^6}{72}I_5\right]\\&+\epsilon^3\left[-\frac{x^7}{14}I_6-\frac{x^8}{60}I_7-\frac{x^9}{1296}I_8\right]\\&+\epsilon^4\left[\frac{x^9}{18}I_8+\frac{71x^{10}}{4200}I_9+\frac{x^{11}}{720}I_{10}+\frac{x^{12}}{31104}I_{11}\right]+\cdots\end{aligned} \tag{8.7}$$

$$\begin{aligned}\Gamma_0=K_1&+\epsilon\left[\frac{x^3}{6}K_2\right]+\epsilon^2\left[-\frac{x^5}{10}K_4+\frac{x^6}{72}K_5\right]\\&+\epsilon^3\left[\frac{x^7}{14}K_6-\frac{x^8}{60}K_7+\frac{x^9}{1296}K_8\right]\\&+\epsilon^4\left[-\frac{x^9}{18}K_8+\frac{71x^{10}}{4200}K_9-\frac{x^{11}}{720}K_{10}+\frac{x^{12}}{31104}K_{11}\right]+\cdots\end{aligned} \tag{8.8}$$

$$\begin{aligned}M_0=I_0&-\epsilon\left[x^2I_2+\frac{x^3}{6}I_3\right]+\epsilon^2\left[x^4I_4+\frac{4}{15}x^5I_5+\frac{x^6}{72}I_6\right]\\&-\epsilon^3\left[x^6I_6+\frac{71}{210}x^7I_7+\frac{11}{360}x^8I_8+\frac{x^9}{1296}I_9\right]\\&+\epsilon^4\left[x^8I_8+\frac{124}{315}x^9I_9+\frac{299}{6300}x^{10}I_{10}\right.\\&\left.+\frac{7}{3240}x^{11}I_{11}+\frac{x^{12}}{31104}I_{12}\right]-\cdots\end{aligned} \tag{8.9}$$

[13] G. Breit and M. H. Hull, Jr., Phys. Rev. **80**, 392 (1950).
[14] G. Breit and M. H. Hull, Jr., Phys. Rev. **80**, 561 (1950).
[15] M. Abramowitz, Quart. Appl. Math. **7**, 75 (1949).
[16] M. Abramowitz, J. Math. Phys. **29**, 303 (1950).
[17] M. Abramowitz, J. Math. Phys. **33**, 111 (1954).

$$N_0=-K_0+\epsilon\left[x^2K_2-\frac{x^3}{6}K_3\right]$$
$$+\epsilon^2\left[-x^4K_4+\frac{4}{15}x^5K_5-\frac{x^6}{72}K_6\right]$$
$$+\epsilon^3\left[x^6K_6-\frac{71}{210}x^7K_7+\frac{11}{360}x^8K_8-\frac{x^9}{1296}K_9\right]$$
$$+\epsilon^4\left[-x^8K_8+\frac{124}{315}x^9K_9-\frac{299}{6300}x^{10}K_{10}+\frac{7}{3240}x^{11}K_{11}-\frac{x^{12}}{31104}K_{12}\right]+\cdots. \quad (8.10)$$

Here I_n and K_n stand for $I_n(x)$ and $K_n(x)$, respectively. As is easily found, the Wronskian relation takes the form:

$$M_0\Gamma_0-\Lambda_0N_0\equiv 1/x. \quad (8.11)$$

These formulas look very attractive, but there are some disadvantages which make them less useful. First: only I_0, I_1, K_0, and K_1 are tabulated so far, and all the other functions must be computed by the usual recurrence relations. Second: the present table[18] runs from $x=0$ to $x=10$, and thereby we have the restriction $8\eta\rho\leq 100$. But the region defined by this inequality is completely included in region A, where the power series expansion can be used conveniently. Thus we conclude that formulas (8.7)–(8.10) should be used in this form only occasionally.

If $x>10$ one must turn to the asymptotic expansions for I_n and K_n (see, e.g., reference 18, p. 271). Then it is possible to derive series expressions containing positive and negative powers of x where the coefficients are power series in ϵ. The calculations are straightforward and we only give the result.

Put

$$\begin{cases} a=\sum a_rx^r \\ b=\sum(-1)^ra_rx^r \\ c=\sum(r-1)a_rx^r \\ d=\sum(-1)^r(r-1)a_rx^r \end{cases} \quad (8.12)$$

where the summation is extended over a suitable number of terms: $r=0, \pm1, \pm2, \cdots$. The coefficients a_r are given below.

$$\begin{cases}
a_0=1-0.051269531\epsilon-0.135408014\epsilon^2-1.23451242\epsilon^3-23.0925\epsilon^4-\cdots \\
a_1=-0.13671875\epsilon-0.250589848\epsilon^2-1.977075\epsilon^3-33.8186\epsilon^4-\cdots \\
a_2=0.3125\epsilon+0.469676971\epsilon^2+3.5501813\epsilon^3+59.45395\epsilon^4+\cdots \\
a_3=-0.166666667\epsilon-0.34777832\epsilon^2-2.66566868\epsilon^3-44.86142\epsilon^4-\cdots \\
a_4=0.1900390625\epsilon^2+1.43372623\epsilon^3+24.03583\epsilon^4+\cdots \\
a_5=-0.071875\epsilon^2-0.58281662\epsilon^3-9.88621\epsilon^4-\cdots \\
a_6=0.0138888889\epsilon^2+0.1831962\epsilon^3+3.25853\epsilon^4+\cdots \\
a_7=-0.0448624545\epsilon^3-0.88331286\epsilon^4-\cdots \\
a_8=0.00792824074\epsilon^3+0.197876088\epsilon^4+\cdots \\
a_9=-0.000771604938\epsilon^3-0.03625545\epsilon^4-\cdots \\
a_{10}=0.0052594\epsilon^4+\cdots \\
a_{11}=-0.00055218\epsilon^4+\cdots \\
a_{12}=0.0000321502\epsilon^4+\cdots \\
a_{-1}=-0.375-0.052871704\epsilon-0.2059647\epsilon^2-2.29335\epsilon^3-49.24\epsilon^4-\cdots \\
a_{-2}=-0.1171875-0.08591652\epsilon-0.4835767\epsilon^2-6.680154\epsilon^3-\cdots \\
a_{-3}=-0.1025390625-0.187942386\epsilon-1.482806\epsilon^2-25.36398\epsilon^3-\cdots \\
a_{-4}=-0.1441955567-0.513485447\epsilon-5.512588\epsilon^2-\cdots \\
a_{-5}=-0.27757645-1.6768509\epsilon-23.85393\epsilon^2-\cdots \\
a_{-6}=-0.67659259-6.35806\epsilon-99.1941\epsilon^2-\cdots \\
a_{-7}=-1.99353173-27.4191\epsilon-\cdots \\
a_{-8}=-6.8839143-132.422\epsilon-\cdots \\
a_{-9}=-27.248827-707.630\epsilon-\cdots \\
a_{-10}=-121.59789-4143.717\epsilon-\cdots \\
a_{-11}=-603.844-\cdots \\
a_{-12}=-3302.27-\cdots.
\end{cases} \quad (8.13)$$

Then we have:

$$\begin{cases} \Lambda_0=e^x(2\pi x)^{-\frac{1}{2}}\cdot a \\ M_0=e^x(2\pi x)^{-\frac{1}{2}}\cdot\{(1+3/2x)a+c/x\} \\ \Gamma_0=e^{-x}(\pi/2x)^{\frac{1}{2}}\cdot b \\ N_0=e^{-x}(\pi/2x)^{\frac{1}{2}}\cdot\{(-1+3/2x)b+d/x\} \end{cases} \quad (8.14)$$

and from these expressions we easily obtain F_0, F_0', G_0, and G_0' according to (8.6). The Wronskian relation can now be written

$$ab+(bc-ad)/2x\equiv 1. \quad (8.15)$$

[18] BAAS, Math. Tables VI, *Bessel Functions*, Part I (Cambridge University Press, London, 1950).

The method just described can be used for values of η greater than $c\cdot\rho^3$ where c is a constant. A reasonable choice seems to be $c=2$. In this way we obtain region B (Fig. 2) determined by

$$\eta>2\rho^3;\quad \eta\rho>50. \tag{8.16}$$

Numerical Example

$$\eta=200,\ \rho=1$$

Thus we have $\epsilon=(16\eta^2)^{-1}=1/640000$ and $x=(8\eta\rho)^{\frac{1}{2}}=40$. We obtain:

$$\begin{cases} a=0.97477751125\\ b=1.02691879721\\ c=-1.01295445465\\ d=-0.98364396653\end{cases}$$

and $ab+(bc-ad)/2x=0.999999999966$. Further we get, e.g., $\phi_0=7.2366047314\cdot10^{14}$ to be compared with $\phi_0=7.2366047313738\cdot10^{14}$ as obtained from the power series.

9. THE RICCATI METHOD

In the ρ-η-plane there are two large regions between the transition region and the regions for small ρ and small η, respectively. For these regions the Riccati method is well suited.

First we consider the case $\rho<2\eta$ (region C), which has been treated in considerable detail by Abramowitz,[15] p. 80. Here we only give the result* with some new terms added, and further we give the expressions for F_0', G_0, and G_0'.

$$\begin{cases} F_0=(1/2)e^{\varphi(t,\eta)}; & F_0'=(2\eta)^{-1}\cdot F_0\cdot d\varphi/dt\\ G_0=e^{\psi(t,\eta)}; & G_0'=(2\eta)^{-1}\cdot G_0\cdot d\psi/dt.\end{cases} \tag{9.1}$$

Here $t=\rho/2\eta$ and

$$\begin{cases} \varphi(t,\eta)=2\eta\cdot g_0+g_1+(2\eta)^{-1}g_2\\ \qquad\qquad +(2\eta)^{-2}g_3+(2\eta)^{-3}g_4+\cdots\\ \psi(t,\eta)=-2\eta\cdot g_0+g_1-(2\eta)^{-1}g_2\\ \qquad\qquad +(2\eta)^{-2}g_3-(2\eta)^{-3}g_4+\cdots\end{cases} \tag{9.2}$$

$$\begin{cases} g_0=[t(1-t)]^{1/2}+\arcsin\sqrt{t}-\pi/2\\ g_1=(1/4)\cdot\log\{t/(1-t)\}\\ g_2=-(8t^2-12t+9)/48t^{1/2}(1-t)^{3/2}\\ g_3=(8t-3)/64t(1-t)^3\\ g_4=\dfrac{2048t^6-9216t^5+16128t^4-13440t^3-12240t^2+7560t-1890}{92160t^{3/2}(1-t)^{9/2}}\\ g_5=3(1024t^3-448t^2+208t-39)/8192t^2(1-t)^6\\ g_6=-(262144t^{10}-1966080t^9+6389760t^8-11714560t^7+13178880t^6-9225216t^5+13520640t^4\\ \quad -3588480t^3+2487240t^2-873180t+130977)/10321920t^{5/2}(1-t)^{15/2}\\ g_7=\dfrac{1105920t^5-55296t^4+314624t^3-159552t^2+45576t-5697}{393216t^3(1-t)^9}\end{cases} \tag{9.3}$$

$$\begin{cases} g_0'=t^{-1/2}(1-t)^{1/2}\\ g_1'=1/4t(1-t)\\ g_2'=-(8t-3)/32t^{3/2}(1-t)^{5/2}\\ g_3'=3(8t^2-4t+1)/64t^2(1-t)^4\\ g_4'=-(1536t^3-704t^2+336t-63)/2048t^{5/2}(1-t)^{11/2}\\ g_5'=3(2560t^4-832t^3+728t^2-260t+39)/4096t^3(1-t)^7\\ g_6'=\dfrac{-368640t^5-30720t^4+114944t^3-57792t^2+16632t-2079}{65536t^{7/2}(1-t)^{17/2}}\\ g_7'=\dfrac{3(860160t^6+196608t^5+308480t^4-177280t^3+73432t^2-17724t+1899)}{131072t^4(1-t)^{10}}.\end{cases} \tag{9.4}$$

* We take the opportunity to correct an error in reference 15, Eqs. (4.5) and (4.6), where the denominator of g_2 should read $12\rho(2\eta-\rho)$ instead of $12\eta(2\eta-\rho)$.

In (9.3) g_0 differs from the corresponding value of reference 15, Eq. (4.5) by the term $-\pi/2$. This is due to the constant $C_0=(2\pi\eta/(e^{2\pi\eta}-1))^{1/2}\simeq e^{-\pi\eta}\cdot(2\pi\eta)^{1/2}$ which has been included. (The approximation above is valid to 13 digits, if $\eta\geq 5$.)

It is clear that this method should be useful if η is sufficiently large and ρ not too close to 0 or 2η. A closer investigation gives the region C (Fig. 2), where the limits must not be looked upon as well-defined. However it turns out that the accuracy is very sensitive to small changes in t close to the line III with the equation: $\eta=3\rho/5+3$. For higher values of η the line IV $3\eta=2\rho+1$ can be used instead.

Numerical Examples

I. $\eta=5, \rho=10$. This point lies on the line I, and therefore we try the power series expansion and the Riccati method.

$$\begin{cases} F_0=1.7207453\cdot 10^{-6} & \text{(Riccati)} \\ F_0=1.7207454\cdot 10^{-6} & \text{(Power series)} \\ F_0=1.7208\cdot 10^{-6} & \text{(Table (reference 12), computed from } F_5\text{)}. \end{cases}$$

II. $\eta=100$, $\rho=4$. This point is situated in C but rather close to region B.

$$\begin{cases} \phi_0=5.7229844\cdot 10^{21} & \text{(Riccati)} \\ \phi_0=5.722993\cdot 10^{21} & \text{(Bessel-Clifford)} \\ \phi_0=5.722985155\cdot 10^{21} & \text{(Power series)}. \end{cases}$$

III. $\eta=\rho=10$.

$$\begin{cases} F_0=1.626275\cdot 10^{-3} & \text{(Riccati)} \\ F_0=1.626\cdot 10^{-3} & \text{(Table (reference 12), } F_0\text{)} \\ F_0=1.6262711\cdot 10^{-3} & \text{(Table (reference 12), from } F_5\text{)} \\ F_0=1.62627115\cdot 10^{-3} & \text{(Power series)}. \end{cases}$$

Now we turn to the region G which has also been treated by Abramowitz[15] in some detail. However, we will use a slightly modified method. Starting from Eq. (2.1) we first perform the transformation:

$$x=2\eta/\rho;\quad y=e^{f(x)}$$

from which we obtain:

$$f''+f'^2+2f'/x+4\eta^2(1-x)/x^4=0.$$

Then we expand $f(x)$ as before:

$$f(x)=2\eta\cdot g_0+g_1+(2\eta)^{-1}g_2+(2\eta)^{-2}g_3+\cdots$$

and obtain the following system of equations:

$$\begin{cases} g_0'^2+(1-x)/x^4=0 \\ g_0''+2g_0'g_1'+(2/x)\cdot g_0'=0 \\ g_1''+g_1'^2+2g_0'g_2'+(2/x)\cdot g_1'=0 \\ g_2''+2g_0'g_3'+2g_1'g_2'+(2/x)\cdot g_2'=0 \\ \cdots\cdots\cdots \end{cases} \tag{9.5}$$

Now we know that when $\rho\to\infty$, i.e., $x\to 0$, the amplitude of F_0 and $G_0\to 1$ and the phase tends to the value

$$\theta_0=\rho-\eta\log 2\rho+\sigma_0.$$

If we use the asymptotic expression for σ_0 (reference 3, p. XXVI) we get

$$\theta_0\sim\rho-\eta\log 2\rho+\frac{\pi}{4}+\eta\log\eta-\eta$$
$$-1/12\eta-1/360\eta^3-1/1260\eta^5-\cdots. \tag{9.6}$$

The integration constants must be determined so as to meet these conditions. We easily find that $g_1, g_3, g_5, \cdots$ are real, and thus we have: $g_1(0)=g_3(0)=g_5(0)=\cdots=0$. $g_0, g_2, g_4, \cdots$ turn out to be purely imaginary, and $(1/i)\cdot(2g_0+(2\eta)^{-1}g_2+(2\eta)^{-3}g_4+\cdots)$ should go over into θ_0 when $x\to 0$. This condition accounts for the negative sign of g_0' and for the constant term $i\pi/8\eta$ in g_0. Further we must have $(1/i)(2\eta)^{-1}g_2(0)=-1/12\eta$, $(1/i)(2\eta)^{-3}g_4(0)=-1/360\eta^3$ and so on. These conditions happen to be fulfilled without special precautions.

In this way we obtain

$$\begin{cases} g_0=i\{(1-x)^{1/2}/x+(1/2)\log\{[1-(1-x)^{1/2}]/[1+(1-x)^{1/2}]\}+\pi/8\eta\} \\ g_0'=-i(1-x)^{1/2}/x^2 \\ g_1=-(1/4)\log(1-x) \\ g_1'=1/4(1-x) \\ g_2=-i(9x^2-12x+8)/48(1-x)^{3/2} \\ g_2'=-i(8x-3x^2)/32(1-x)^{5/2} \\ g_3=-(8x^3-3x^4)/64(1-x)^3 \\ g_3'=-3(8x^2-4x^3+x^4)/64(1-x)^4 \\ \cdots\cdots\cdots \end{cases}$$

We write the result in the following form:

$$\begin{cases} M=\{1/(1-x)\}^{1/4}\cdot e^{\psi(\eta,x)} \\ \psi(\eta,x)=-(8x^3-3x^4)/64(2\eta)^2(1-x)^3+3x^5(1024-448x+208x^2-39x^3)/8192(2\eta)^4(1-x)^6 \\ \qquad -\dfrac{x^7(1105920-55296x+314624x^2-159552x^3+45576x^4-5697x^5)}{393216(2\eta)^6(1-x)^9}+\cdots \\ \varphi(\eta,x)=2\eta\left(\dfrac{(1-x)^{1/2}}{x}+\dfrac{1}{2}\log\dfrac{1-(1-x)^{1/2}}{1+(1-x)^{1/2}}\right)+\dfrac{\pi}{4}-(9x^2-12x+8)/48(2\eta)(1-x)^{3/2} \\ \qquad -\dfrac{2048-9216x+16128x^2-13440x^3-12240x^4+7560x^5-1890x^6}{92160(2\eta)^3(1-x)^{9/2}} \\ \qquad -(130977x^{10}-873180x^9+2487240x^8-3588480x^7+13520640x^6-9225216x^5 \\ \qquad +15178880x^4-11714560x^3+6389760x^2-1966080x+262144)/10321920(2\eta)^5(1-x)^{15/2}-\cdots. \end{cases} \tag{9.6}$$

Of course, the coefficients in this expansion are the same as in (9.3). Further we put:

$$\begin{cases} A(\eta,x)=(1-x)^{1/2}/x^2+(8x-3x^2)/32(2\eta)^2(1-x)^{5/2}-x^3(1536-704x+336x^2-63x^3)/2048(2\eta)^4(1-x)^{11/2} \\ \qquad +\dfrac{x^5(368640-30720x+114944x^2-57792x^3+16632x^4-2079x^5)}{65536\cdot(2\eta)^6\cdot(1-x)^{17/2}}-\cdots \\ B(\eta,x)=1/4(2\eta)(1-x)-3x^2(x^2-4x+8)/64(2\eta)^3(1-x)^4 \\ \qquad +3x^4(2560-832x+728x^2-260x^3+39x^4)/4096(2\eta)^5(1-x)^7 \\ \qquad -\dfrac{3x^6(1899x^6-17724x^5+73432x^4-177280x^3+308480x^2+196608x+860160)}{131072(2\eta)^7(1-x)^{10}}+\cdots. \end{cases} \tag{9.7}$$

Then we have the final result

$$\begin{cases} F_0=M\cdot\sin\varphi \\ G_0=M\cdot\cos\varphi \\ F_0'=-x^2(BF_0-AG_0) \\ G_0'=-x^2(AF_0+BG_0) \end{cases} \tag{9.8}$$

with the Wronskian relation

$$AM^2x^2\equiv1. \tag{9.9}$$

Numerical examples will be given later.

10. ASYMPTOTIC EXPANSIONS ON THE TRANSITION LINE

In reference 8 Abramowitz and Rabinowitz, starting from an integral representation by Newton, have obtained some very useful expressions for the functions F_0, G_0, F_0', G_0' when $\rho=2\eta$, and they also give a small table of the functional values for $\rho=0(0.5)20(2)50$. In a more recent work by Biedenharn, Gluckstern, Hull, and Breit[19] these formulas have been generalized to the case $L>0$. The convergence in this case, however, is rather slow, unless L is small and η large. Here we restrict ourselves to $L=0$ and write down the same formulas as in reference 8 with some more terms added, using the compact notation of reference 19.

$$\begin{Bmatrix} F_0(2\eta) \\ G_0(2\eta)/\sqrt{3} \end{Bmatrix}\cong\frac{\Gamma(1/3)\beta^{1/2}}{2\sqrt{\pi}}\left\{1\mp\frac{2}{35}\cdot\frac{\Gamma(2/3)}{\Gamma(1/3)}\cdot\frac{1}{\beta^4}-\frac{32}{8100}\cdot\frac{1}{\beta^6}\mp\frac{92672}{7371\cdot10^4}\cdot\frac{\Gamma(2/3)}{\Gamma(1/3)}\cdot\frac{1}{\beta^{10}}-\frac{6363008}{3536379\cdot10^4}\cdot\frac{1}{\beta^{12}}\right.$$
$$\left.\mp\frac{391911498752}{679377699\cdot10^7}\cdot\frac{\Gamma(2/3)}{\Gamma(1/3)}\cdot\frac{1}{\beta^{16}}\cdots\right\} \tag{10.1}$$

[19] Biedenharn, Gluckstern, Hull, and Breit, Phys. Rev. **97**, 542 (1955).

$$\begin{Bmatrix} F_0'(2\eta) \\ G_0'(2\eta)/\sqrt{3} \end{Bmatrix} \cong \frac{\Gamma(2/3)}{2\sqrt{\pi}\cdot\beta^{1/2}} \left\{ \pm 1 + \frac{1}{15}\frac{\Gamma(1/3)}{\Gamma(2/3)}\cdot\frac{1}{\beta^2} \pm \frac{8}{56700}\cdot\frac{1}{\beta^6} + \frac{11488}{18711\cdot 10^3}\cdot\frac{\Gamma(1/3)}{\Gamma(2/3)}\cdot\frac{1}{\beta^8} \pm \frac{25739264}{4179357\cdot 10^5}\cdot\frac{1}{\beta^{12}} + \frac{1246983424}{180355329\cdot 10^5}\cdot\frac{\Gamma(1/3)}{\Gamma(2/3)}\cdot\frac{1}{\beta^{14}} \pm \cdots \right\}. \quad (10.2)$$

Here $\beta=(2\eta/3)^{1/3}$; $\Gamma(1/3)=2.6789385347$ and $\Gamma(2/3)=1.3541179394$.

Following reference 8 we also give the formulas in a form suitable for numerical computation.

$$\begin{Bmatrix} F_0(2\eta) \\ G_0(2\eta) \end{Bmatrix} \cong \begin{Bmatrix} 0.7063326373 \\ 1.223404016 \end{Bmatrix} \cdot \eta^{1/6} \cdot \left\{ 1 \mp \frac{0.04959570165}{\eta^{4/3}} - \frac{0.008888888889}{\eta^2} \mp \frac{0.002455199181}{\eta^{10/3}} - \frac{0.0009108958061}{\eta^4} \mp \frac{0.0002534684115}{\eta^{16/3}} - \cdots \right\} \quad (10.3)$$

$$\begin{Bmatrix} F_0'(2\eta) \\ G_0'(2\eta) \end{Bmatrix} \cong \begin{Bmatrix} 0.4086957323 \\ -0.7078817734 \end{Bmatrix} \cdot \eta^{-1/6} \cdot \left\{ 1 \pm \frac{0.1728260369}{\eta^{2/3}} + \frac{0.0003174603174}{\eta^2} \pm \frac{0.003581214850}{\eta^{8/3}} + \frac{0.0003117824680}{\eta^4} \pm \frac{0.0009073966427}{\eta^{14/3}} + \cdots \right\}. \quad (10.4)$$

Numerical Example

Already for $\eta=1$ we obtain an accuracy of 0.1%. For $\rho=10$, $\eta=5$ we get:

$$\begin{cases} F_0=0.9179450 & \text{(Formula (10.3))} \\ F_0=0.9179449 & \text{(reference 8, Table I).} \end{cases}$$

11. EXPANSIONS IN TERMS OF AIRY INTEGRALS

As is well known it is rather difficult to compute Coulomb wave functions in the transition region with a fair accuracy. One possibility is to use numerical quadrature as indicated in Sec. 5, and another to compute a key value on the transition line as described in Sec. 10 and then integrate Eq. (2.1) numerically. Both these methods are in general rather time consuming, especially for large values of η.

It has been pointed out by Abramowitz and Antosiewics[20] that it is possible to obtain F_0 and G_0 in terms of Airy integrals. They also discuss briefly how to proceed when $L>0$. However, this special method has some disadvantages. First, the convergence, even for moderate values of the argument, is very slow. Second, the formula involves a set of constants which must be determined by reference to the functional values on the transition line.†

The paper by Biedenharn, Gluckstern, Hull, and Breit[19] which gives much useful information on Coulomb wave functions, especially for higher values of L, also contains expansions in terms of usual and modified Bessel functions of orders $\pm n/3$, and these functions appear in such a way as to be expressible in terms of Airy integrals. However, the expansions, obtained by using a Green's function for solving a system of nonhomogeneous differential equations, are rather difficult to construct, and it seems practically prohibitive to proceed beyond the first two terms.

As has been shown by Tyson[21] and by Feshbach, Shapiro, and Weisskopf,[22] a straightforward expansion in terms of Airy integrals can be obtained directly from the differential equation in the case $L=0$, and it is easy to see that this method has none of the disadvantages just mentioned. Starting with the Eq. (2.1) for $L=0$, and following reference 20 we put $x=(2\eta-\rho)/(2\eta)^{1/3}$; $\mu=(2\eta)^{2/3}$ to obtain

$$y''-\mu xy/(\mu-x)=0. \quad (11.1)$$

Now we try the following expansion:

$$y=\text{const}\{Ai(x)\cdot(1+g_1(x)/\mu+g_2(x)/\mu^2+\cdots) + Ai'(x)\cdot(f_1(x)/\mu+f_2(x)\mu^2+\cdots)\}. \quad (11.2)$$

Then we easily find the conditions:

$$\begin{cases} f_n''(x)+2g_n'(x)=\sum_{k=0}^{n-1} x^{n-k+1}f_k(x) \\ g_n''(x)+2xf_n'(x)+f_n(x)=\sum_{k=0}^{n-1} x^{n-k+1}g_k(x) \end{cases} \quad (11.3)$$

where $f_0(x)\equiv 0$, $g_0(x)\equiv 1$. These equations can be written in the following more practical way:

$$\begin{cases} f_n''+2g_n'=x(f_{n-1}''+2g_{n-1}'+xf_{n-1}) \\ g_n''+2xf_n'+f_n=x(g_{n-1}''+2xf_{n-1}'+f_{n-1}+xg_{n-1}). \end{cases} \quad (11.4)$$

[20] M. Abramowitz and H. A. Antosiewics, Phys. Rev. 96, 75 (1954).

† We take the opportunity to correct a printing error in reference 20, p. 76, Eq. (15), where a minus sign should be placed before the term $y'(0,\mu)Ai(0)$ in the expressions for c_1 and c_2.

[21] J. K. Tyson, Dissertation, Massachusetts Institute of Technology, 1948.

[22] Feshbach, Shapiro, and Weisskopf, NYO 3077, NDA Report 15B-5.

The first functions are:

$$
\left\{
\begin{aligned}
& f_1(x)=x^2/5 \qquad\qquad g_1(x)=-x/5 \\
& f_2(x)=(2x^3+6)/35 \qquad\qquad g_2(x)=x^2(7x^3-30)/350 \\
& f_3(x)=x(84x^6+1480x^3+2320)/63000 \qquad\qquad g_3(x)=(1056x^6-1160x^3-2240)/63000 \\
& f_4(x)=x^2(1254x^6+9952x^3+11488)/693000 \\
& g_4(x)=x(3234x^9+621280x^6-478800x^3-804160)/48510000 \\
& f_5(x)=\frac{168168x^{12}+118209520x^9+610662080x^6+713574400x^3+2140723200}{63063\cdot 10^6} \\
& g_5(x)=\frac{x^2(2666664x^9+210254720x^6-138044480x^3-356787200)}{21021\cdot 10^6} \\
& f_6(x)=\frac{x(2858856x^{12}+788972288x^9+3064641024x^6+3407716480x^3+8635845120)}{441441\cdot 10^6} \\
& g_6(x)=(3531528x^{15}+6633266640x^{12}+317451563200x^9-183526546560x^6 \\
& \qquad\qquad -388613030400x^3-579033728000)/3972969\cdot 10^7 \\
& f_7(x)=x^2(17153136x^{15}+69192483360x^{12}+11135701248640x^9+35219971257600x^6 \\
& \qquad\qquad +40263767308800x^3+113475491584000)/67540473\cdot 10^8 \\
& g_7(x)=x(1783926144x^{15}+1283288054880x^{12}+43988924714240x^9-23231154374400x^6 \\
& \qquad\qquad -55484432640000x^3-113475491584000)/67540473\cdot 10^8.
\end{aligned}
\right.
\tag{11.5}
$$

The constant can easily be determined by putting $x=0$; then the expansion goes over into formula (10.1), and we have a possibility to check (10.1) and (11.5) against each other.‡

The final result is

$$
\left\{
\begin{aligned}
& F_0=\pi^{1/2}(2\eta)^{1/6}\cdot\{Ai(x)(1+g_1/\mu+g_2/\mu^2+\cdots)+Ai'(x)(f_1/\mu+f_2/\mu^2+\cdots)\} \\
& G_0=\pi^{1/2}(2\eta)^{1/6}\cdot\{Bi(x)(1+g_1/\mu+g_2/\mu^2+\cdots)+Bi'(x)(f_1/\mu+f_2/\mu^2+\cdots)\} \\
& F_0'=-\pi^{1/2}(2\eta)^{-1/6}\cdot\{Ai(x)[(g_1'+xf_1)/\mu+(g_2'+xf_2)/\mu^2+\cdots] \\
& \qquad\qquad +Ai'(x)[1+(g_1+f_1')/\mu+(g_2+f_2')/\mu^2+\cdots]\} \\
& G_0'=-\pi^{1/2}(2\eta)^{-1/6}\cdot\{Bi(x)[(g_1'+xf_1)/\mu+(g_2'+xf_2)/\mu^2+\cdots] \\
& \qquad\qquad +Bi'(x)[1+(g_1+f_1')/\mu+(g_2+f_2')/\mu^2+\cdots]\}.
\end{aligned}
\right.
\tag{11.6}
$$

The functions $Ai(x)$, $Ai'(x)$, $Bi(x)$, and $Bi'(x)$ are tabulated.[23] It should be observed that the formulas above can be used for both positive and negative values of x.

The Wronskian relation can be written:

$$
\begin{aligned}
(1+g_1/\mu+g_2/\mu^2+\cdots)[1+(g_1+f_1')/\mu & \\
+(g_2+f_2')/\mu^2+\cdots] & \\
-(f_1/\mu+f_2/\mu^2+\cdots)[(g_1'+xf_1)/\mu & \\
+(g_2'+xf_2)/\mu^2+\cdots]\equiv 1 &
\end{aligned}
\tag{11.7}
$$

and from this identity a number of checking relations can be obtained. The first ones of them are

$$f_1'+g_1\equiv 0.$$

$$f_2'+2g_2+f_1'g_1+g_1^2-f_1g_1'-xf_1^2\equiv 0.$$

$$f_3'+2g_3+f_2'g_1+2g_1g_2+f_1'g_2-f_1g_2'-2xf_1f_2-f_2g_1'\equiv 0.$$

The formulas (11.6) can be used in region E with about 5 digits accuracy or better.

Numerical Examples

I. $\rho=120$, $\eta=50$.

$$\left\{\begin{aligned} F_0&=0.200255 \\ G_0&=1.55061\end{aligned}\right. \quad \text{(Airy)}$$

$$\left\{\begin{aligned} F_0&=0.200254 \\ G_0&=1.55060\end{aligned}\right. \quad \text{(Riccati, (9.8))}$$

‡ If we put $L=0$ in Eqs. (24) and (25), reference 19, we should obtain the first terms in (11.6). A discrepancy in sign seems to indicate a minor error in reference 19.

[23] BAAS, Math. Tables, Part-Volume B, *The Airy Integral*, prepared by J. C. P. Miller (Cambridge University Press, London, 1946).

II. $\rho=80$, $\eta=50$.

$$\begin{cases} F_0=0.001203665 & \text{(Airy)} \\ F_0=0.001203655 & \text{(Riccati, (9.1))} \end{cases}$$

III. $\rho=10$, $\eta=4$.

$$\begin{cases} F_0=1.3992085 & \text{(Airy)} \\ F_0=1.39921 & \text{(Table 12)} \end{cases}$$

The points (120, 50) and (80, 50) are very hard to reach, indeed; nevertheless our semiconvergent expansions give quite accurate results.

Note.—The terms in (11.6) vary in a very regular way, and by using a logarithmic extrapolation, one can obtain at least two more terms approximately and gain considerably in accuracy.

12. ASYMPTOTIC EXPANSION FOR LARGE VALUES OF ρ

In this section we again admit $L\geq 0$. When ρ is large compared with η and L, it is possible to derive asymptotic expressions for the Coulomb wave functions. In reference 3 Abramowitz has obtained such formulas using the integral representation. Here we will instead start from Eq. (2.1). First we perform the transformation $y=u\cdot e^{i\theta_L}$ where

$$\theta_L=\rho-\eta\log 2\rho-\frac{L}{2}\pi+\sigma_L$$

and

$$\sigma_L=\arg\Gamma(i\eta+L+1)=\arg\Gamma(i\eta+1)+\sum_{k=1}^{L}\mathrm{arctg}(\eta/k).$$

Then we get the equation

$$u''+2i(1-\eta/\rho)u' +\{i\eta(1+i\eta)-L(L+1)\}\cdot u/\rho^2=0. \quad (12.1)$$

Now we put $u=u_0+u_1+u_2+\cdots$ with $u_n=a_n/\rho^n$ and obtain:

$$a_{n+1}/a_n=(i\eta-L+n)(i\eta+L+n+1)/2i(n+1). \quad (12.2)$$

We split u_n into its real and imaginary part

$$u_n=s_n+it_n$$

and further we introduce:

$$A_n=(2n+1)\cdot\eta/2(n+1)\rho;$$

$$B_n=\{L(L+1)-n(n+1)+\eta^2\}/2(n+1)\rho.$$

Then we find the recursion formulas:

$$\begin{cases} s_{n+1}=A_n s_n-B_n t_n \\ t_{n+1}=A_n t_n+B_n s_n \end{cases} \quad (12.3)$$

For computation of the derivatives we put

$$\begin{cases} S_n=s_n'-t_n(1-\eta/\rho) \\ T_n=t_n'+s_n(1-\eta/\rho) \end{cases} \text{ to obtain:}$$

$$\begin{cases} S_{n+1}=A_n S_n-B_n T_n-s_{n+1}/\rho \\ T_{n+1}=A_n T_n+B_n S_n-t_{n+1}/\rho. \end{cases} \quad (12.4)$$

As is easily found from the known behavior at infinity we have the following initial conditions:

$$s_0=1,\quad t_0=0,\quad S_0=0,\quad T_0=1-\eta/\rho. \quad (12.5)$$

Now we put

$$s=\sum s_n;\quad t=\sum t_n;\quad S=\sum S_n;\quad T=\sum T_n \quad (12.6)$$

where the summation of the divergent series is cut off after a suitable number of terms (i.e., when the wanted accuracy has been obtained or when the terms of the series start to increase again). Putting $\theta_L=\theta$ we get the final result:

$$\begin{cases} F_L=t\cdot\cos\theta+s\cdot\sin\theta \\ G_L=s\cdot\cos\theta-t\cdot\sin\theta \\ F_L'=T\cdot\cos\theta+S\cdot\sin\theta \\ G_L'=S\cdot\cos\theta-T\cdot\sin\theta \end{cases} \quad (12.7)$$

with the Wronskian relation

$$sT-St\equiv 1. \quad (12.8)$$

This method can be used when $\eta^2\ll\rho$ and when $L^2\ll\rho$. In the case $L=0$ a closer investigation gives the region H (Fig. 2) as result.

Numerical Examples

I. $\rho=50$, $\eta=9$.

$$\begin{cases} F_0=0.93570855 \\ G_0=-0.61180203 \end{cases} \text{(Riccati, (9.8))}$$

$$\begin{cases} F_0=0.935709 \\ G_0=-0.611802 \end{cases} \begin{matrix}\text{(Asymptotic formula, (12.7);} \\ \text{only 6 decimals carried)}\end{matrix}$$

II. $\rho=20$, $\eta=5$.

$$\begin{cases} F_0=-0.229352 \\ G_0=1.165712 \end{cases} \text{(Riccati, (9.8))}$$

$$\begin{cases} F_0=-0.229347 \\ G_0=1.165716 \end{cases} \text{(As. formula, (12.7))}$$

II. $\rho=10$, $\eta=3$.

$$\begin{cases} F_0=0.660103 \\ G_0=-1.060141 \end{cases} \text{(As. formula, (12.7))}$$

$$\begin{cases} F_0=0.660099 \\ G_0=-1.06011 \end{cases} \text{(Table 12)}$$

13. CONCLUSION

It is obvious that many more methods for computation of Coulomb wave functions exist, and even some quite satisfactory methods have not been mentioned here. However, we have tried to avoid such methods as are dependent on other functions than the elementary ones, for quite obvious reasons. For example, the expansions in terms of spherical Bessel functions (due to P. M. Morse) and usual Bessel functions (Abramowitz) (see reference 3, p. XVIII) have not been discussed. There are a few exceptions from this rule: we have referred to the tables in references 3 and 12 which seems legitimate, and to the table of Airy integrals, since these functions can hardly be avoided.

When numerical values of Coulomb wave functions are needed, then Figs. 1 and 2 which are self-explanatory, first should be consulted. For convenience we give Table I. (When $\rho,\eta\leq 10$, consult Fig. 1 in Sec. 4.) We also give the equations of the curves in Fig. 2.

I. $\eta\rho=50$

II. $\eta=2\rho^3$

III. $\eta=3\rho/5+3$

IV. $3\eta=2\rho+1$

V. $2\eta=\rho$

VI. $\eta=2\rho/5$

VII. $\eta=13\rho/30-5/2$

VIII. $\eta^2+4\eta+3=12\rho/5$.

TABLE I.

Region	Method	Reference
A	Power series	(7.7, 12)
B	Bessel-Clifford	(8.6, 14)
C	Riccati I	(9.1)
D	Quadrature or num. integration	(5.2, 5)
E	Airy integrals	(11.6)
F	Special case of E $(x=0)$	(10.3, 4)
G	Riccati II	(9.8)
H	Asymptotic formula	(12.7)

It is obvious that these curves must not be looked upon as limits which cannot be exceeded. In many cases two and even three methods overlap, and this gives a good possibility to check the computations.

14. REMARKS ON FUTURE TABLES

From the discussion above it can be concluded that when future tables are being prepared one should concentrate on a region formed by a parallelogram with its corners in $(\rho,\eta)=(10,0)$, $(20,5)$, $(20,15)$, and $(10,10)$. The table should be constructed as a "skeleton table" with e.g., $L=0,5,10$ and $\Delta\rho=1$, $\Delta\eta=1/2$. At the same time the table (reference 12) should be enlarged so that $\Delta\eta=1/2$ instead of 1. The region mentioned here seems to be the most difficult (and most important!) one at the time present. As far as can be judged, numerical quadrature will be adequate in the whole region, and no special complications should be expected.